

# EIC 1700 SEARCH REQUEST

SCIENTIFIC REFERENCE BR  
Sci & Tech Inf. Cntr.

Today's Date

3-18-2008

MAR 20 REC'D

Pat. &amp; T.M. Office

Name

Sin J. Lee

Priority App. Filing Date

P.B. attached

AU/Org.

1795

Examiner #

76060

Case/App. #

10/589,382

Bld.&amp;Rm.#

9C15  
(Rem.)

Phone

2-1333

Format for Search Results

EMAIL

PAPER

If this is a Board of Appeals case, check here ☐

Synonyms

Describe this invention in your own words.

Terms to avoid

**Additional Comments**

Plz. search for the compound  
of cl. # 1 wherein  
the "malonic ester residue"  
has the formula (I)  
in cl. # 2.

Please submit completed form to your EIC. SPE Signature here indicates Rush

## STAFF USE ONLY

## Type of Search

## Vendors and cost where applicable

Searcher:

MH

NA Sequence (#)

STN

Searcher Phone #:

AA Sequence (#)

Dialog

Searcher Location:

Structure (#)

Questel/Orbit

Date Searcher Picked Up:

Bibliographic

Dr.Link

Date Completed:

3/31/08

Litigation

Lexis/Nexis

Searcher Prep &amp; Review Time:

Fulltext

Sequence Systems

Clerical Prep Time:

Patent Family

WWW/Internet

Online Time:

Other

Other (specify)



## UNITED STATES PATENT AND TRADEMARK OFFICE

UNITED STATES DEPARTMENT OF COMMERCE  
 United States Patent and Trademark Office  
 Address: COMMISSIONER FOR PATENTS  
 P.O. Box 1450  
 Alexandria, Virginia 22313-1450  
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## BIB DATA SHEET

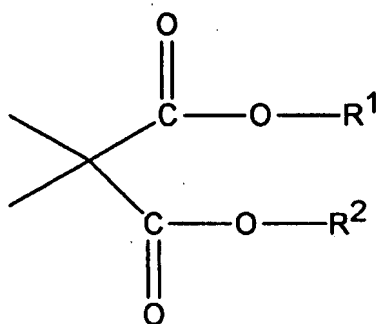
CONFIRMATION NO. 6030

<b>SERIAL NUMBER</b> 10/589,382	<b>FILING or 371(c) DATE</b> 08/15/2006 <b>RULE</b>	<b>CLASS</b> 430	<b>GROUP ART UNIT</b> 1795	<b>ATTORNEY DOCKET NO.</b> 1608-6 PCT/US	
<b>APPLICANTS</b> Toshiyuki Ogata, Kanagawa, JAPAN; Takuma Hojo, Kanagawa, JAPAN; Hiromitsu Tsuji, Kanagawa, JAPAN; Takako Hirosaki, Kanagawa, JAPAN; Mitsuru Sato, Kanagawa, JAPAN; <b>** CONTINUING DATA *****</b> This application is a 371 of PCT/JP05/01392 02/01/2005 <b>** FOREIGN APPLICATIONS *****</b> JAPAN 2004-043692 02/19/2004 <b>** IF REQUIRED, FOREIGN FILING LICENSE GRANTED **</b> 05/07/2007					
Foreign Priority claimed <input type="checkbox"/> Yes <input type="checkbox"/> No 35 USC 119(a-d) conditions met <input type="checkbox"/> Yes <input type="checkbox"/> No Verified and Acknowledged <input type="checkbox"/> Met after Allowance Examiner's Signature _____ Initials _____		<b>STATE OR COUNTRY</b> JAPAN	<b>SHEETS DRAWINGS</b> 0	<b>TOTAL CLAIMS</b> 11	<b>INDEPENDENT CLAIMS</b> 1
<b>ADDRESS</b> HOFFMANN & BARON, LLP 6900 JERICHO TURNPIKE SYOSSET, NY 11791 UNITED STATES					
<b>TITLE</b> Photoresist composition and method of forming resist pattern					
<b>FILING FEE RECEIVED</b> 900	FEES: Authority has been given in Paper No. _____ to charge/credit DEPOSIT ACCOUNT No. _____ for following:		<input type="checkbox"/> All Fees		
			<input type="checkbox"/> 1.16 Fees (Filing)		
			<input type="checkbox"/> 1.17 Fees (Processing Ext. of time)		
			<input type="checkbox"/> 1.18 Fees (Issue)		
			<input type="checkbox"/> Other _____		
			<input type="checkbox"/> Credit		

## CLAIMS

1. A photoresist composition, comprising: a fullerene derivative (A) having two or more malonic ester residues.

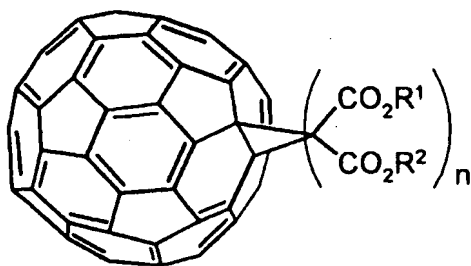
2. The photoresist composition according to Claim 1, wherein the malonic ester residue is the group expressed by the general formula (1) below,



(1)

in which,  $\text{R}^1$  and  $\text{R}^2$  independently represent an alkyl group, which may be identical or different from each other.

3. The photoresist composition according to Claim 1, in which the fullerene derivative (A) is a compound, expressed by the general formula (2) below,



(2)

in which,  $n$  is an integer of 2 or more, and  $R^1$  and  $R^2$  independently represent an alkyl group, which may be identical or different from each other.

4. The photoresist composition according to Claim 3, wherein the alkyl group has a normal or branched chain, or cyclic alkyl group having 1 to 10 carbons, and  $n$  is an integer from 2 to 10.

5. The photoresist composition according to Claim 1, comprising the fullerene derivative (A), a radiation sensitive acid generator (B), and an organic solvent.

6. The photoresist composition according to Claim 5, further comprising a film forming resin component (C).

7. The photoresist composition according to Claim 6, wherein the photoresist composition is positive-type, and the film formation resin component (C) has an acid-dissociative dissolution-controlling group, which is a resin (C1) that increases solubility to alkali by acid action.

8. The photoresist composition according to Claim 6, wherein the photoresist composition is negative-type, the component (C) is an alkaline soluble resin (C2) and a crosslinking agent component (D).

# VOLUNTARY SEARCH FEEDBACK

Art Unit \_\_\_\_\_

App./Serial # \_\_\_\_\_

## **Relevant prior art found**

- ☐ 102 rejection
- ☐ 103 rejection
- ☐ Cited as being of interest
- ☐ Helped better understand invention
- ☐ Helped better understand state of the art in technology

Types ☐ Foreign Patent(s) ☐ Non-Patent Literature

## **Relevant prior art not found**

- ☐ Results verified the lack of relevant prior art (helped determine patentability).
- ☐ Results were not useful in determining the patentability or understanding of the invention.

## **COMMENTS**

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Questions about the scope or the results of the search?

Contact your EIC searcher or Team Leader.

Please submit completed form to your EIC

## **STIC USE ONLY**

Today's Date \_\_\_\_\_

12/07

Additional Notes if applicable (please indicate all actions including emails, phone calls, and individuals assisting):

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=> fil reg

FILE 'REGISTRY' ENTERED AT 12:34:26 ON 31 MAR 2008  
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STRUCTURE FILE UPDATES: 30 MAR 2008 HIGHEST RN 1011030-42-4  
DICTIONARY FILE UPDATES: 30 MAR 2008 HIGHEST RN 1011030-42-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

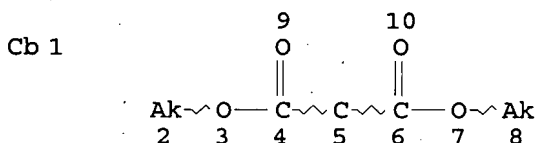
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REGISTRY includes numerically searchable data for experimental and  
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experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> d que stat 17

L5 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM  
GGCAT IS PCY AT 1  
GGCAT IS SAT AT 2  
GGCAT IS SAT AT 8  
DEFAULT ECLEVEL IS LIMITED  
ECOUNT IS M20 C AT 1

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

L7 141 SEA FILE=REGISTRY SSS FUL L5

100.0% PROCESSED 298064 ITERATIONS  
SEARCH TIME: 00.00.04

141 ANSWERS

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FILE 'HCAPLUS' ENTERED AT 12:16:08 ON 31 MAR 2008

E US20070190447/PN  
E WO2005-JP01392/AP  
L1 1 S E3  
SEL RN

FILE 'REGISTRY' ENTERED AT 12:17:22 ON 31 MAR 2008  
L2 12 S E1-12  
L3 25623 S ?FULLERENE?/CNS  
L4 5 S L2 AND L3

FILE 'LREGISTRY' ENTERED AT 12:22:00 ON 31 MAR 2008  
L5 STR

FILE 'REGISTRY' ENTERED AT 12:26:50 ON 31 MAR 2008  
L6 1 S L5  
L7 141 S L5 FUL  
L8 5 S L2 AND L7  
SAV L7 LEE382/A  
L9 136 S L7 NOT L8  
L10 60 S L9 AND L3

FILE 'HCAPLUS' ENTERED AT 12:30:08 ON 31 MAR 2008  
L11 1 S L8  
L12 30 S L10  
L13 QUE MALONIC?  
L14 0 S L12 AND L13  
SEL HIT RN L12  
L15 QUE PHOTORESIST? OR PHOTO(2N)RESIST? OR RESIST OR RESISTS  
L16 0 S L12 AND L15

=> fil hcap

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FILE LAST UPDATED: 30 Mar 2008 (20080330/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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L11 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2005:962524 HCAPLUS

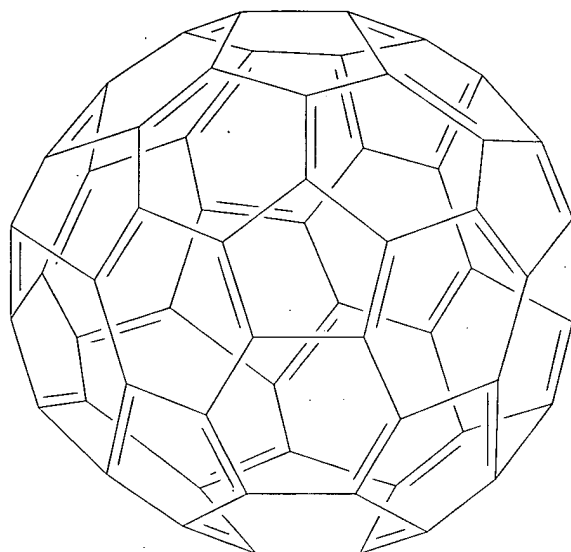
DOCUMENT NUMBER: 143:238698  
 TITLE: Photoresist composition and method of forming resist pattern  
 INVENTOR(S): Ogata, Toshiyuki; Hojo, Takuma; Tsuji, Hiromitsu; Hirosaki, Takako; Sato, Mitsuru  
 PATENT ASSIGNEE(S): Tokyo Ohka Kogyo Co., Ltd.; Japan  
 SOURCE: PCT Int. Appl., 40 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005081061	A1	20050901	WO 2005-JP1392	20050201
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2005266798	A	20050929	JP 2005-41438	20050218
US 20070190447	A1	20070816	US 2006-589382	20060815
KR 2007018033	A	20070213	KR 2006-718377	20060908
PRIORITY APPLN. INFO.:			JP 2004-43692	A 20040219
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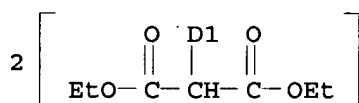
OTHER SOURCE(S): MARPAT 143:238698  
 AB Title photoresist composition contains a fullerene derivative having two or more malonic ester residues for improved etching resistance.  
 IT 862714-07-6P 862714-08-7P 862714-09-8P 862714-10-1P 862714-11-2P  
 RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (photoresist composition containing fullerene malonic ester derivs.)  
 RN 862714-07-6 HCAPLUS  
 CN [5,6]Fullerene-C60-1h-diacetic acid,  $\alpha, \alpha'$ -bis(ethoxycarbonyl)-, diethyl ester (9CI) (CA INDEX NAME)



PAGE 1-A

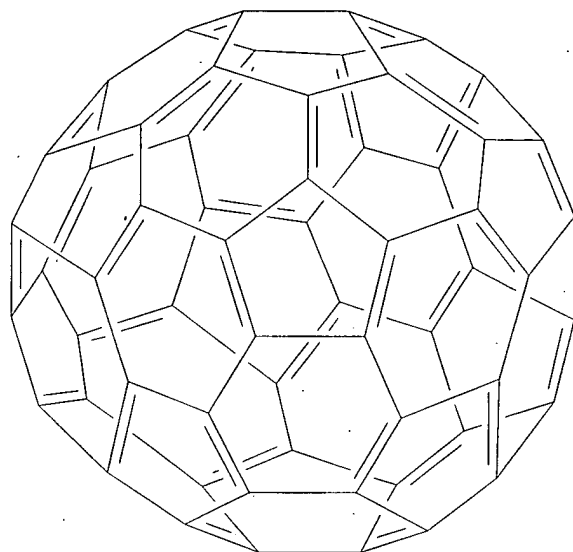


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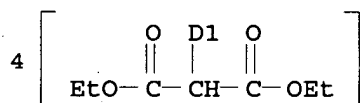


RN 862714-08-7 HCAPLUS  
CN [5,6]Fullerene-C60-1h-tetraacetic acid,  
 $\alpha, \alpha', \alpha'', \alpha'''$ -tetrakis(ethoxycarbonyl)-,  
tetraethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

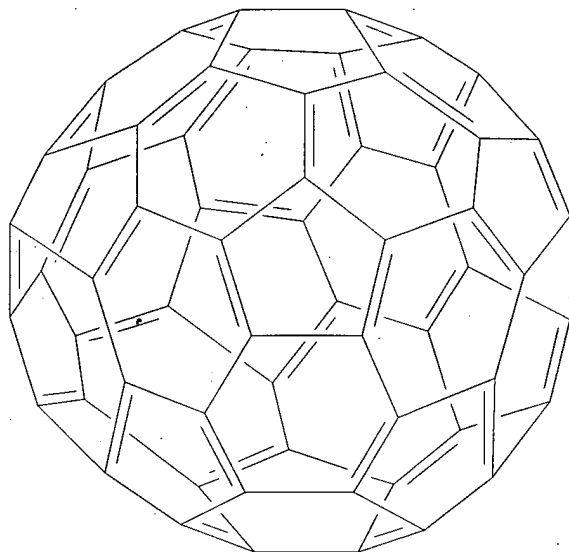


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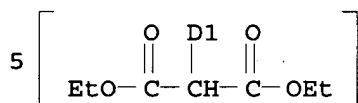


RN 862714-09-8 HCAPLUS  
CN [5,6]Fullerene-C60-1h-pentaacetic acid,  
 $\alpha, \alpha', \alpha'', \alpha''', \alpha''''$ -  
pentakis(ethoxycarbonyl)-, pentaethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



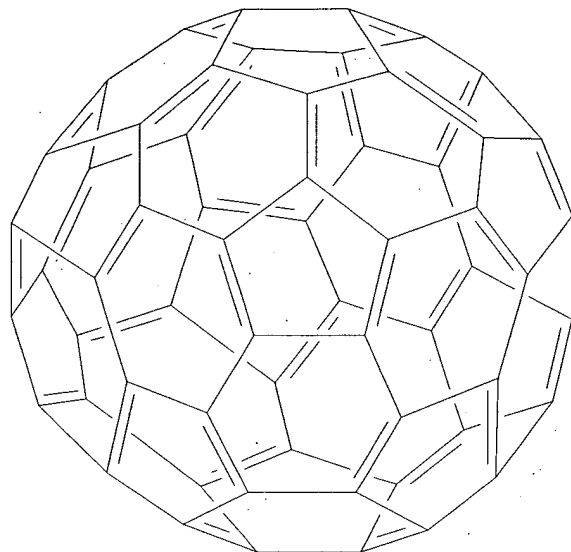
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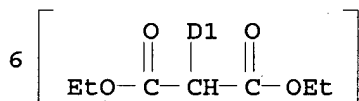
RN 862714-10-1 HCAPLUS

CN [5,6]Fullerene-C60-1h-hexaacetic acid,  $\alpha, \alpha', \alpha'', \alpha''', \alpha'''', \alpha'''''$ -hexakis(ethoxycarbonyl)-, hexaethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

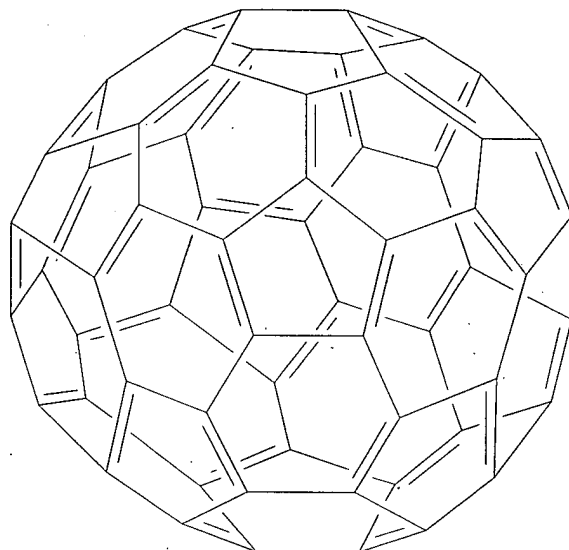


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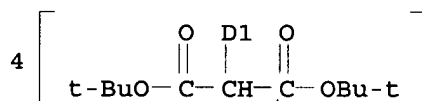


RN 862714-11-2 HCAPLUS  
 CN [5,6]Fullerene-C60-1h-tetraacetic acid,  
 $\alpha, \alpha', \alpha'', \alpha'''$ -tetrakis[(1,1-  
 dimethylethoxy)carbonyl]-, tetrakis(1,1-dimethylethyl) ester (9CI)  
 (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



IC ICM G03F007-004  
 ICS G03F007-038; G03F007-039  
 CC 74-5 (Radiation Chemistry, Photochemistry, and Photographic and  
 Other Reprographic Processes)  
 IT 862714-07-6P 862714-08-7P 862714-09-8P  
 862714-10-1P 862714-11-2P  
 RL: IMF (Industrial manufacture); TEM (Technical or engineered  
 material use); PREP (Preparation); USES (Uses)  
 (photoresist composition containing fullerene malonic ester derivs.)  
 REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR  
 THIS RECORD. ALL CITATIONS AVAILABLE IN  
 THE RE FORMAT

=> d l12 ibib abs hitstr hitind 1-30

L12 ANSWER 1 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:902161 HCAPLUS

DOCUMENT NUMBER: 147:448508

TITLE: Chlorofullerene C60Cl6: A precursor for  
 straightforward preparation of highly  
 water-soluble polycarboxylic fullerene  
 derivatives active against HIV

AUTHOR(S): Troshina, Olesya A.; Troshin, Pavel A.;  
 Peregudov, Alexander S.; Kozlovskiy, Viacheslav  
 I.; Balzarini, Jan; Lyubovskaya, Rimma N.

CORPORATE SOURCE: Institute of Problems of Chemical Physics of  
Russian Academy of Sciences, Chernogolovka,  
142432, Russia

SOURCE: Organic & Biomolecular Chemistry (2007), 5(17),  
2783-2791

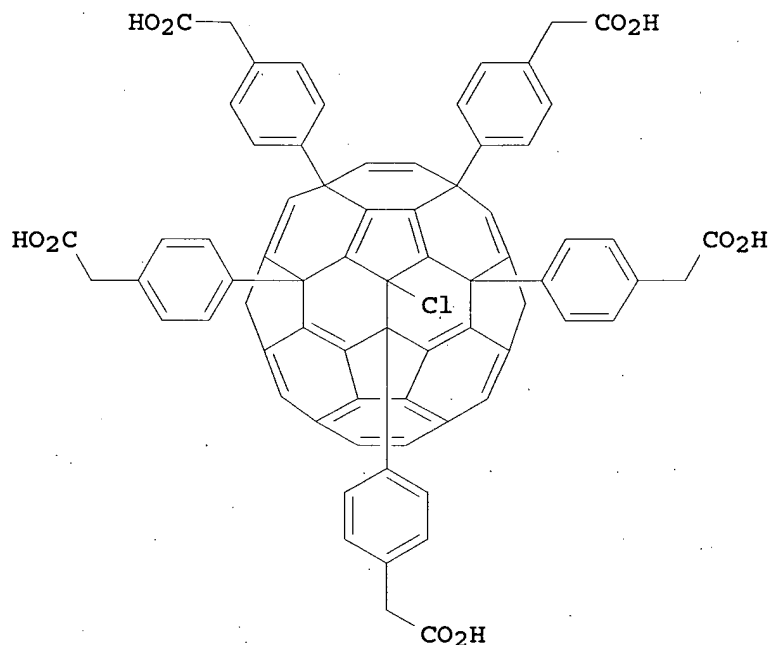
PUBLISHER: CODEN: OBCRAK; ISSN: 1477-0520  
Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 147:448508

GI



AB A hexachlorochlorofullerene  $C_{60}Cl_6$  (I) is prepared regioselectively and chemoselective in 77% yield by chlorination of  $C_{60}$  with iodine monochloride in 1,2-dichlorobenzene; I undergoes regioselective coupling with Me phenylacetate and with di-Me benzylmalonate using ferric chloride in nitrobenzene to give pentaarylchlorofullerenes which are hydrolyzed with trifluoroacetic and hydrochloric acids in aqueous chlorobenzene to give carboxylated pentaarylchlorofullerenes such as II. The potassium salts of carboxylated pentaarylchlorofullerenes such as II are soluble (150-200 mg/mL) in water; the neutral compds. are soluble in DMSO and can be dissolved in water by diluting their DMSO solns. The carboxylated pentaarylchlorofullerene potassium salts are tested as inhibitors of HIV-1 and HIV-2; II has  $EC_{50}$  values of 1.2 and 4.4  $\mu M$  in HIV-1 and HIV-2 infected cells while inhibiting cell growth at  $>63 \mu M$  and  $>14 \mu M$  concns., resp. The carboxylated pentaarylchlorofullerenes are inactive against a variety of other viral species. The nitrobenzene solvent for the regioselective arylation of I is toxic and should be handled with caution.

IT 952156-69-3P

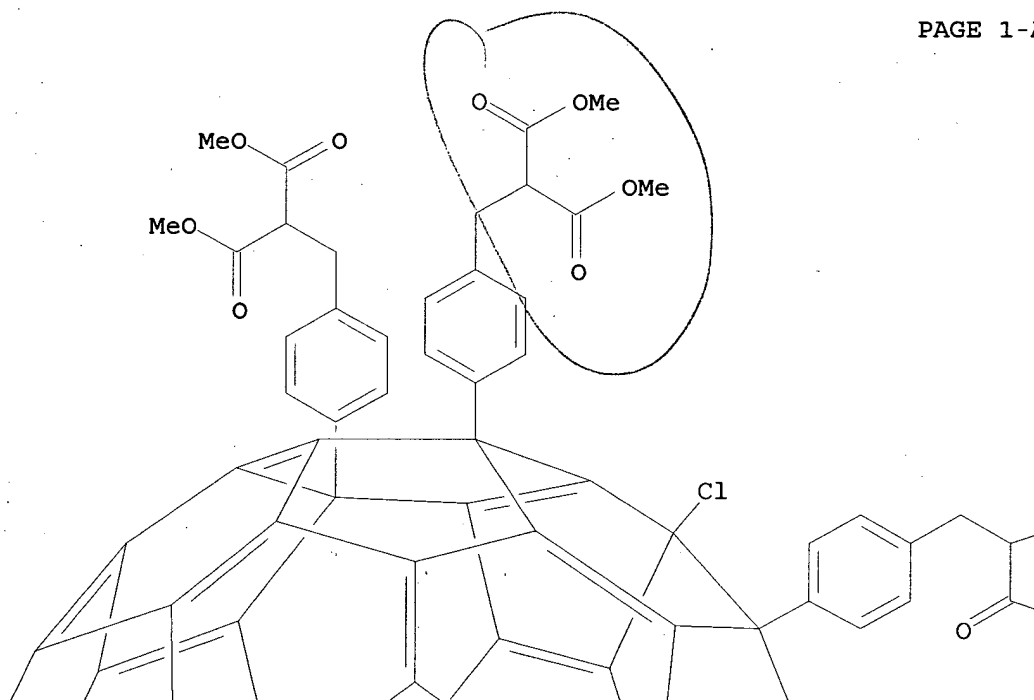
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
RACT (Reactant or reagent)

(preparation of carboxylated pentaarylchlorofullerenes by arylation of  
C60Cl6 and the water solubilities, HIV-1 and HIV-2 inhibition,  
and lack of other antiviral activities of the carboxylated  
pentaarylchlorofullerene potassium salts)

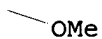
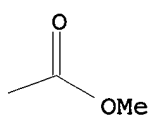
RN 952156-69-3 HCAPLUS

CN Benzenepropanoic acid, 4,4',4'',4''',4''''-(9-chloro[5,6]fullerene-  
C60-1h-1,7,11,24,27(9H)-pentayl)pentakis[ $\alpha$ 1, $\alpha$ 7, $\alpha$ 11  
, $\alpha$ 24, $\alpha$ 27-pentakis(methoxycarbonyl)-,  
1,1',1'',1''',1''''-pentamethyl ester (CA INDEX NAME)

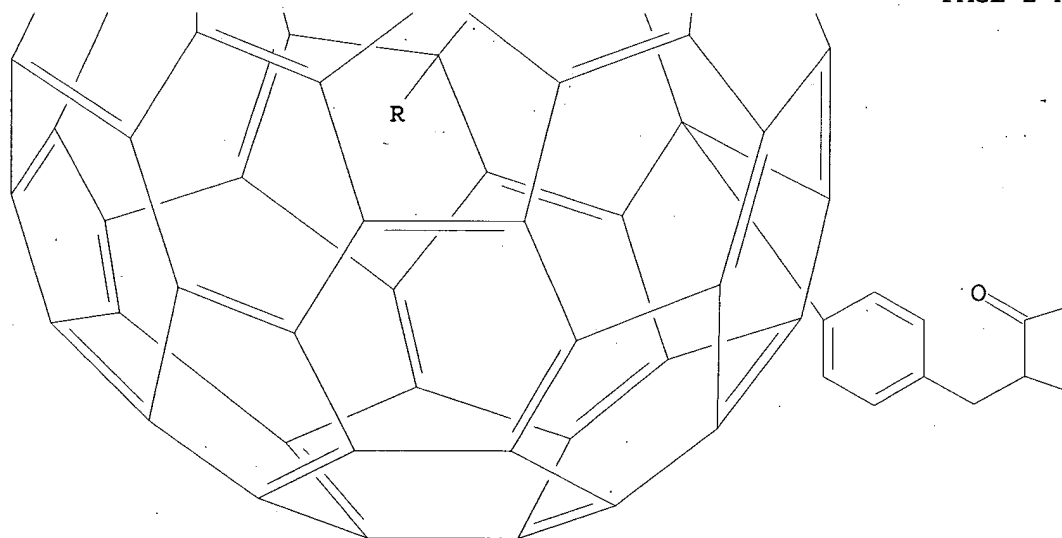
PAGE 1-A



PAGE 1-B

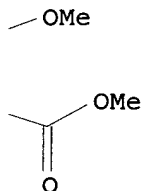


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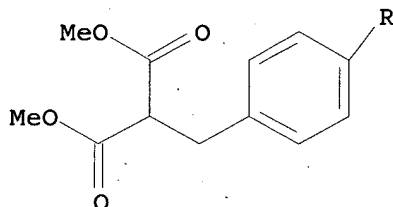




PAGE 2-B



PAGE 3-A



CC 25-29 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds);  
Section cross-reference(s): 1, 10  
IT 952156-68-2P 952156-69-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
RACT (Reactant or reagent)  
(preparation of carboxylated pentaarylchlorofullerenes by arylation of  
C60Cl6 and the water solubilities, HIV-1 and HIV-2 inhibition,  
and lack of other antiviral activities of the carboxylated  
pentaarylchlorofullerene potassium salts)

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE  
FOR THIS RECORD. ALL CITATIONS AVAILABLE  
IN THE RE FORMAT

L12 ANSWER 2 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:443336 HCAPLUS  
DOCUMENT NUMBER: 147:263739  
TITLE: Theoretical investigation for the absorption of  
emerald green [60]fullerenes  
AUTHOR(S): Yin, Yong-yi  
CORPORATE SOURCE: Department of Chemistry, Mudanjiang Teacher's  
College, Mudanjiang, 157012, Peop. Rep. China  
SOURCE: Fenzi Kexue Xuebao (2006), 22(4), 286-288  
CODEN: JMOSE7; ISSN: 1000-9035  
PUBLISHER: Fenzi Kexue Xuebao Bianjibu  
DOCUMENT TYPE: Journal  
LANGUAGE: Chinese

AB The geometry of emerald green [60]fullerenes were optimized by AM1 method. The absorptions of compds. C60[C(CH3)(CO2-t-Bu)2]6 and its derivative with their crystal structures and their optimized structures were calculated at CI-ZINDO level. The calculated maximum absorption wavelength agrees with the exptl. data well.

IT 836649-08-2

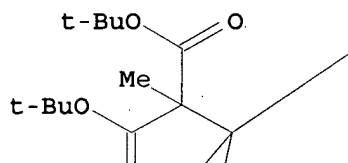
RL: PRP (Properties)

(theor. investigation for optical absorption and electronic structures of emerald green [60]fullerenes)

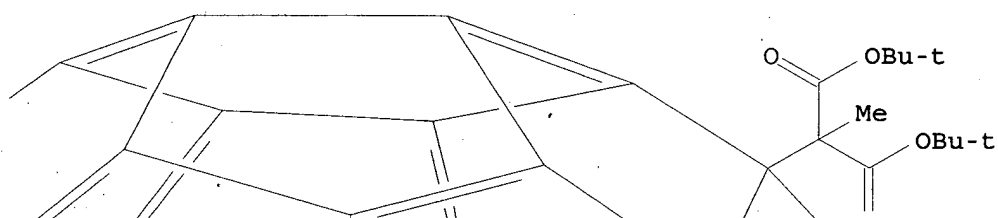
RN 836649-08-2 HCAPLUS

CN [5,6]Fullerene-C60-Ih-1,23,28,33,38,60-hexaacetic acid,  
 $\alpha 1, \alpha 23, \alpha 28, \alpha 33, \alpha 38, \alpha 60$ -  
hexakis[(1,1-dimethylethoxy)carbonyl]- $\alpha 1, \alpha 23, \alpha 28, .$   
 $\alpha 33, \alpha 38, \alpha 60$ -hexamethyl-, 1,23,28,33,38,60-  
hexakis(1,1-dimethylethyl) ester (CA INDEX NAME)

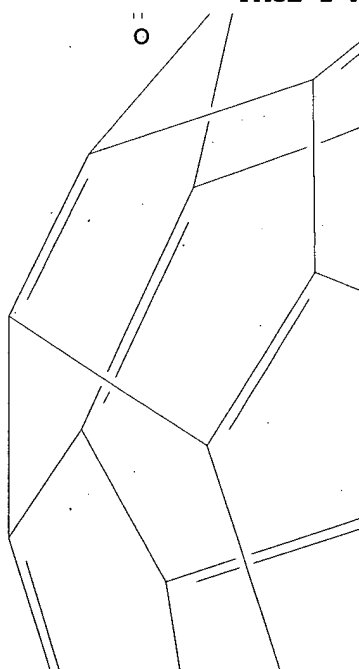
PAGE 1-A



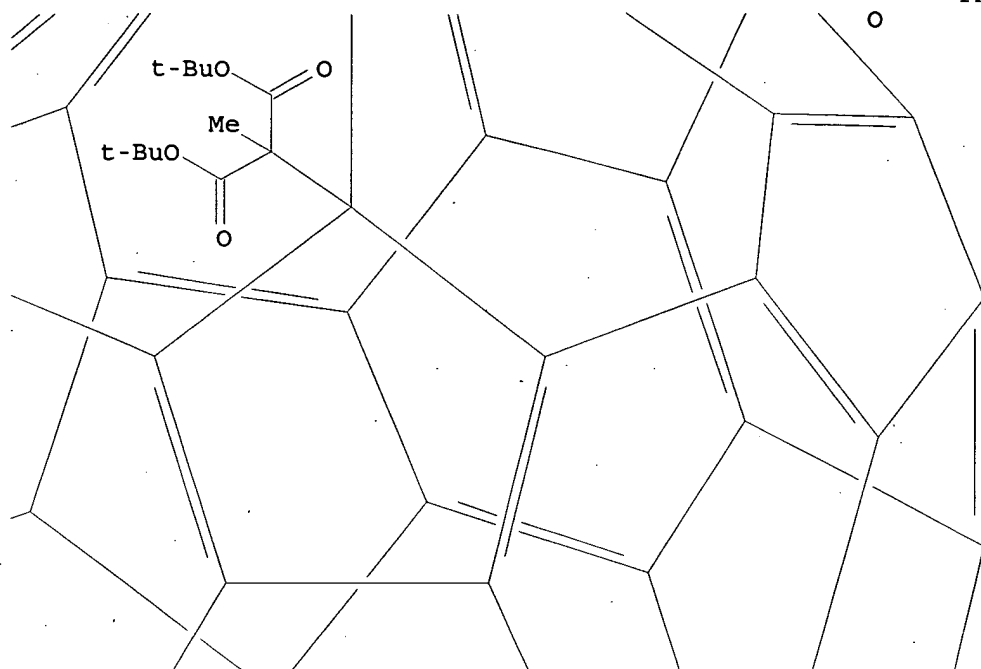
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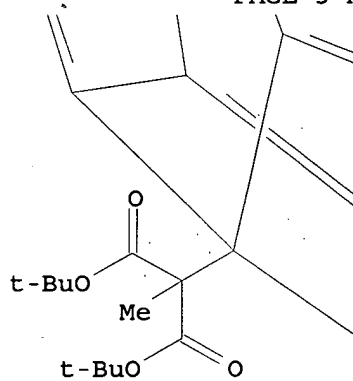
PAGE 2-A



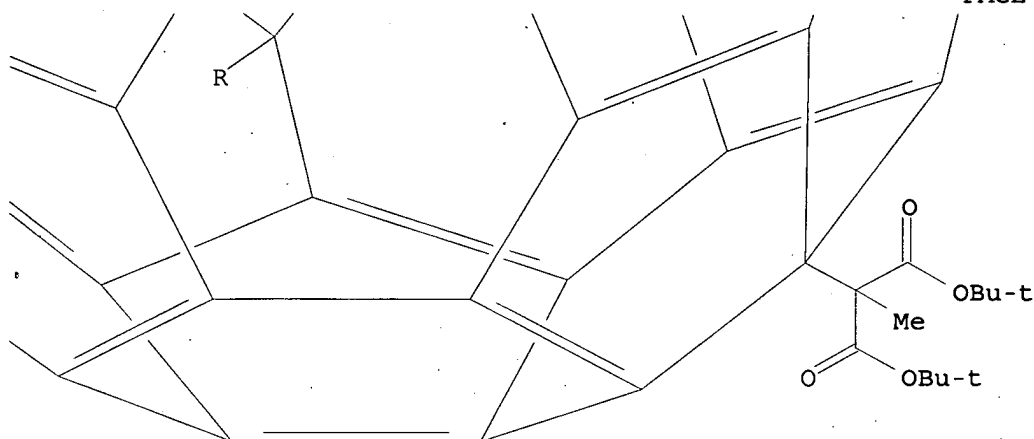
PAGE 2-B



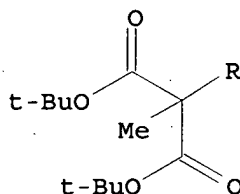
PAGE 3-A



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CC 65-3 (General Physical Chemistry)  
 Section cross-reference(s): 73  
 IT 836649-08-2  
 RL: PRP (Properties)  
 (theor. investigation for optical absorption and electronic  
 structures of emerald green [60]fullerenes)

L12 ANSWER 3 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2006:748198 HCAPLUS  
 DOCUMENT NUMBER: 145:365027  
 TITLE: Low multielectron reduction potentials of  
 emerald green [60]fullerenes  
 AUTHOR(S): Canteenwala, Taizoon; Li, Wenguang; Wang,  
 Hsing-Ling; Chiang, Long Y.  
 CORPORATE SOURCE: Department of Chemistry, University of  
 Massachusetts Lowell, Lowell, MA, 01854, USA  
 SOURCE: Chemistry Letters (2006), 35(7), 762-763  
 CODEN: CMLTAG; ISSN: 0366-7022  
 PUBLISHER: Chemical Society of Japan  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Unique double-triphenylene interconnected all-trans 18-trannulene  
 electronic configuration of dodecaethylated emerald green fullerene  
 (EFn), C60[-CMe(CO2Et)2]6 or EF-6MC2, allows the fullerene cage to  
 retain similar affinity for electrons as C60 and high multielectron  
 accepting capability with E1Red = -0.36 V, E2Red = -0.88 V, and  
 E3Red = -1.45 V vs. Ag/AgCl.

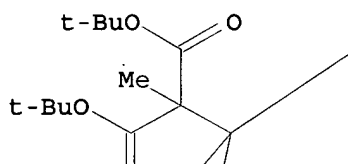
IT 836649-08-2

RL: PRP (Properties)  
(Schlegel diagram of)

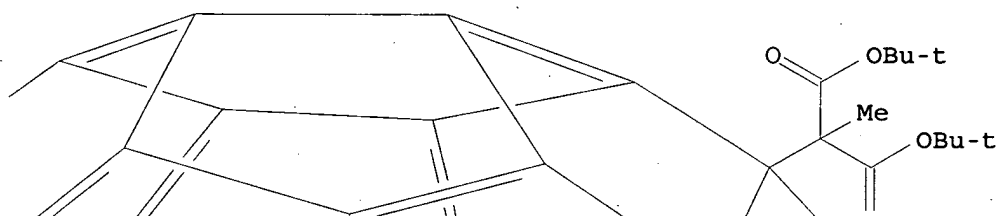
RN 836649-08-2 HCAPLUS

CN [5,6]Fullerene-C60-Ih-1,23,28,33,38,60-hexaacetic acid,  
 $\alpha$ 1, $\alpha$ 23, $\alpha$ 28, $\alpha$ 33, $\alpha$ 38, $\alpha$ 60-  
hexakis[(1,1-dimethylethoxy)carbonyl]- $\alpha$ 1, $\alpha$ 23, $\alpha$ 28,.  
 $\alpha$ 33, $\alpha$ 38, $\alpha$ 60-hexamethyl-, 1,23,28,33,38,60-  
hexakis(1,1-dimethylethyl) ester (CA INDEX NAME)

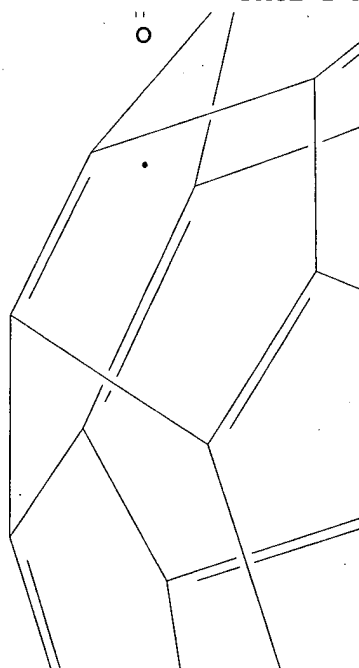
PAGE 1-A



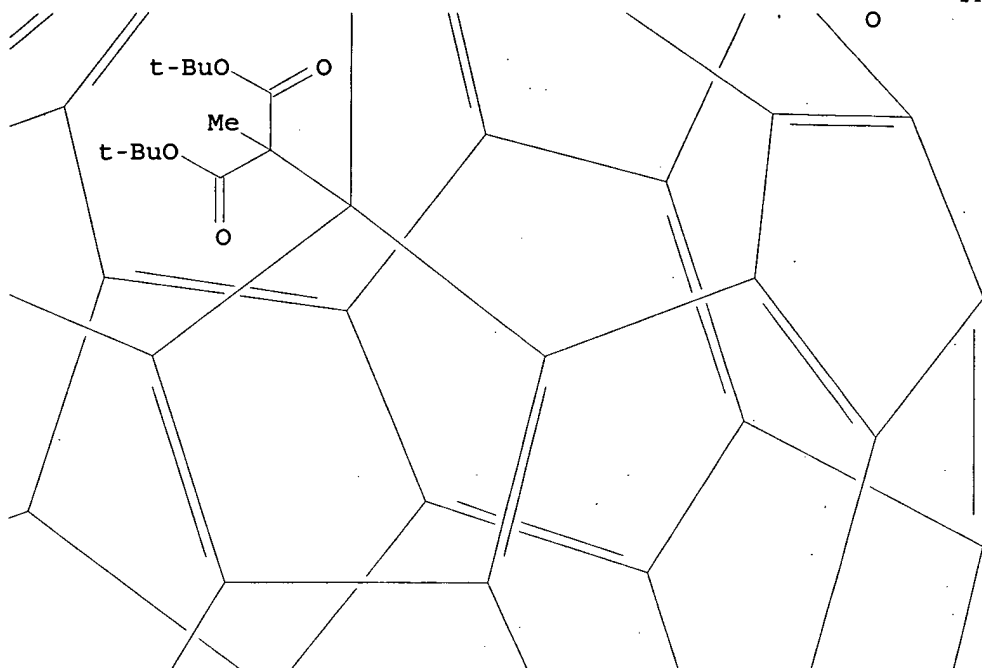
PAGE 1-B



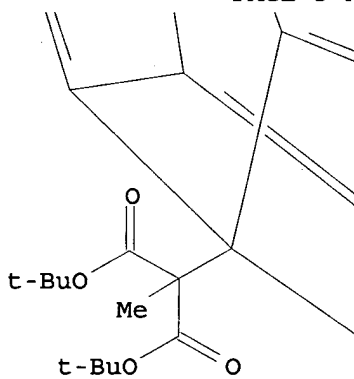
PAGE 2-A



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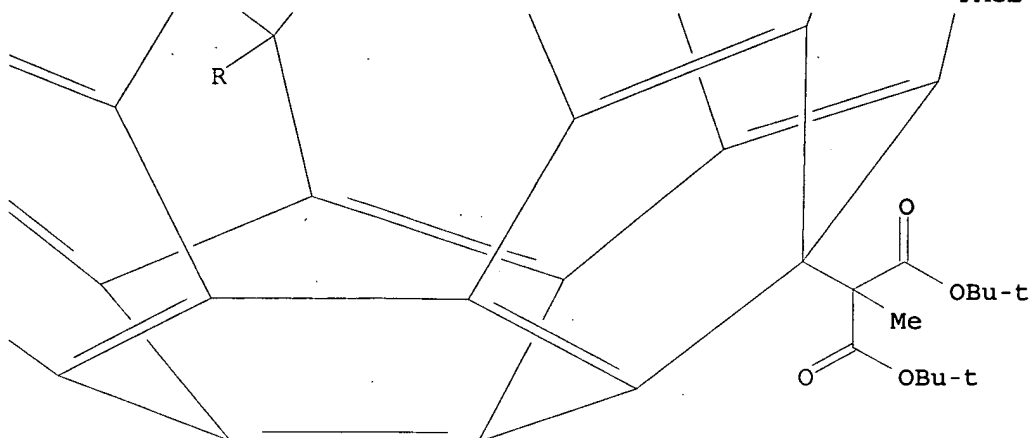


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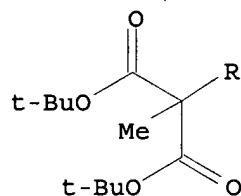




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IT 836649-07-1

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(cyclic voltammetry in THF containing Bu<sub>4</sub>NPF<sub>6</sub> and low multielectron reduction potentials of emerald green [60]fullerenes)

RN 836649-07-1 HCAPLUS

CN [5,6]Fullerene-C60-1h-1,23,28,33,38,60-hexaacetic acid,

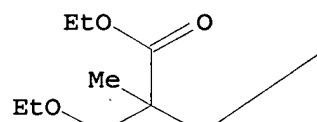
$\alpha, \alpha', \alpha'', \alpha''', \alpha''''$

hexakis(ethoxycarbonyl)- $\alpha, \alpha', \alpha'', \alpha'''$ , .alpha

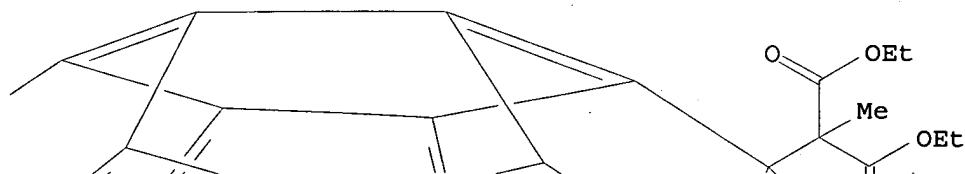
.''''', $\alpha''''''$ -hexamethyl-, hexaethyl ester (9CI) (CA INDEX

NAME)

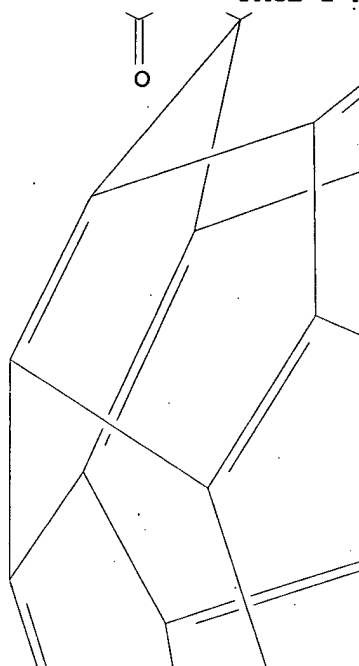
PAGE 1-A



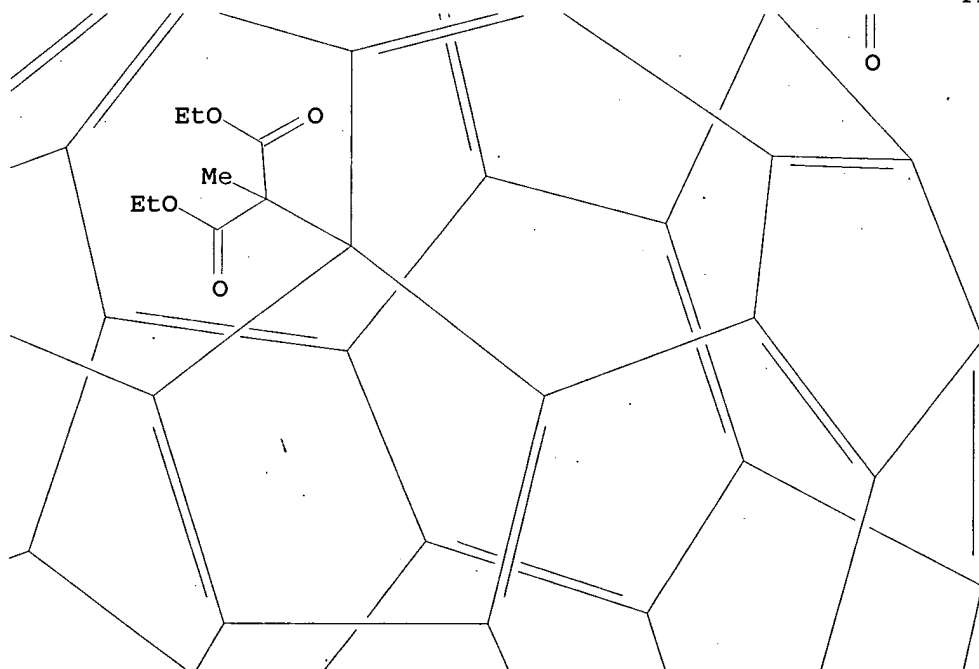
PAGE 1-B



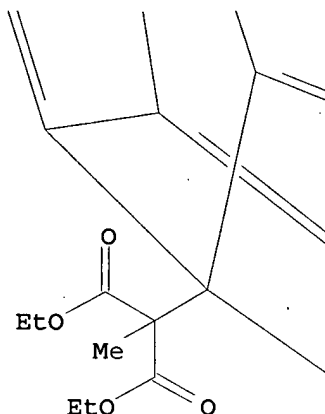
PAGE 2-A



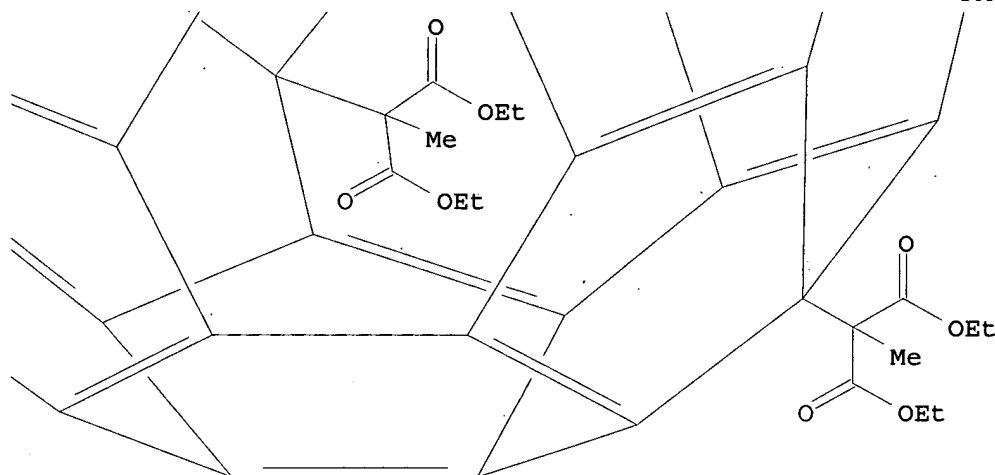
PAGE 2-B



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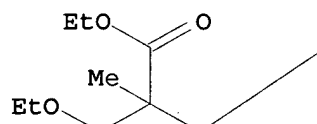
IT 910131-71-4 910134-53-1

RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)  
 (electrochem. reductive formation and electrochem. reduction and reduction potential in THF containing Bu<sub>4</sub>NPF<sub>6</sub>)

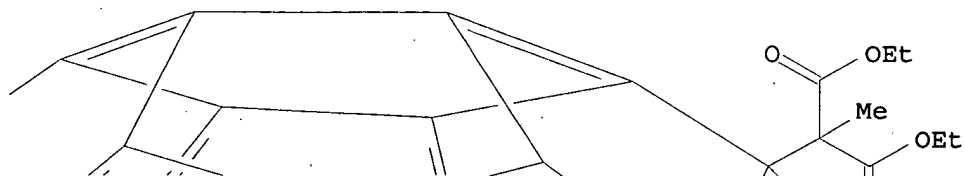
RN 910131-71-4 HCAPLUS

CN [5,6]Fullerene-C60-1h-1,23,28,33,38,60-hexaacetic acid,  
 $\alpha, \alpha', \alpha'', \alpha''', \alpha'''', \alpha'''''$ -  
 hexakis(ethoxycarbonyl)- $\alpha, \alpha', \alpha'', \alpha'''$ , .alpha  
 $\alpha''''', \alpha''''''$ -hexamethyl-, hexaethyl ester, radical ion(1-)  
 (9CI) (CA INDEX NAME)

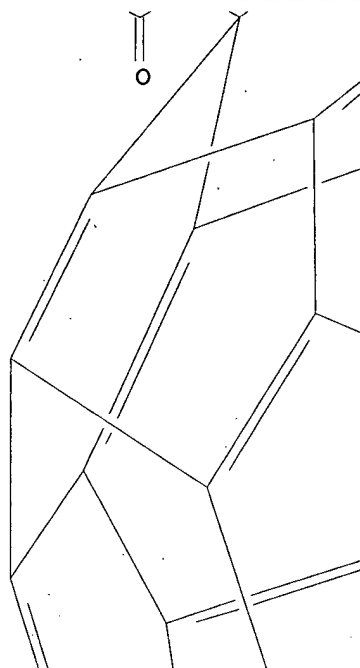
PAGE 1-A



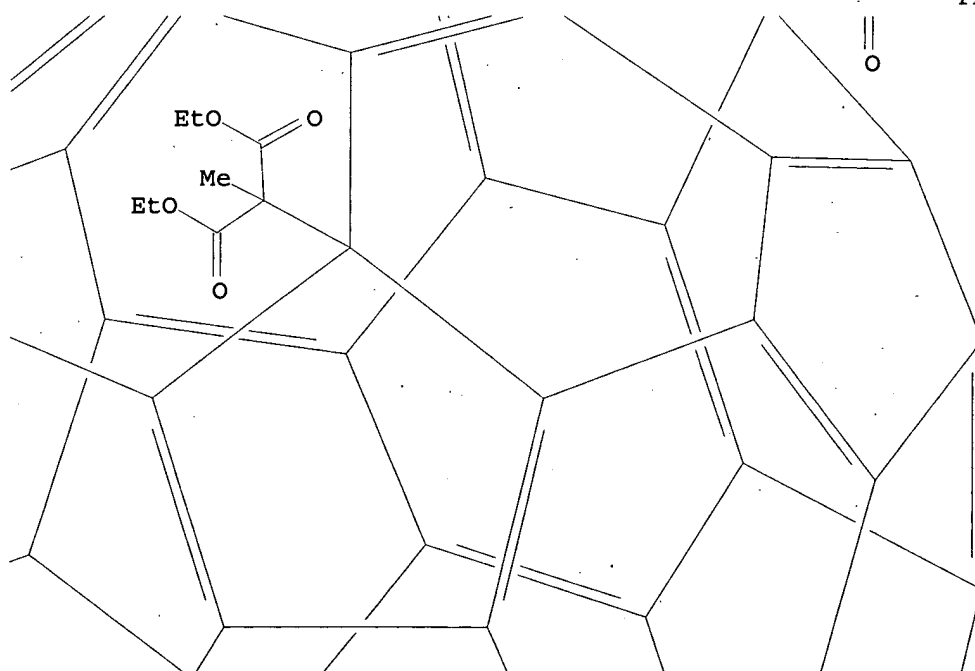
PAGE 1-B



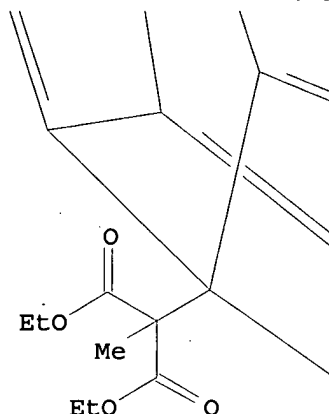
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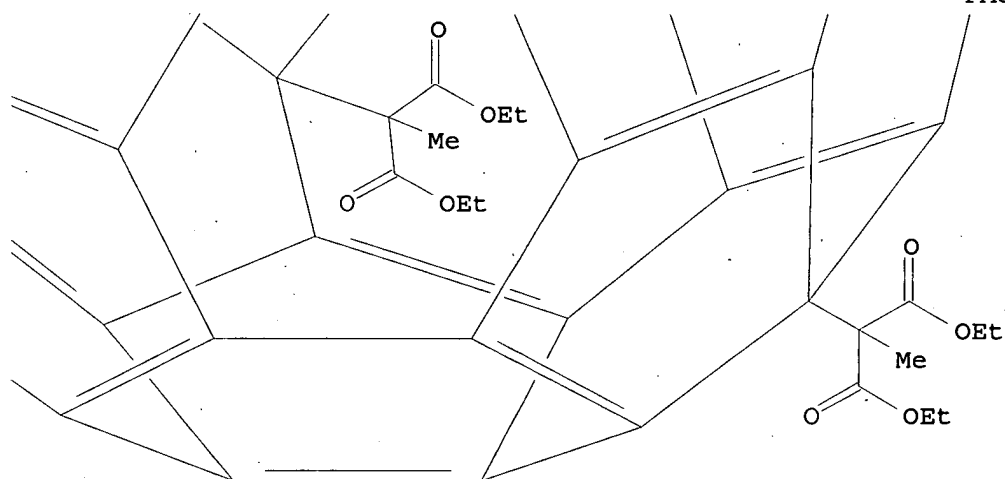
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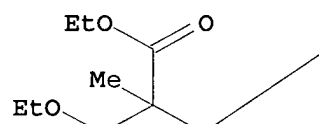


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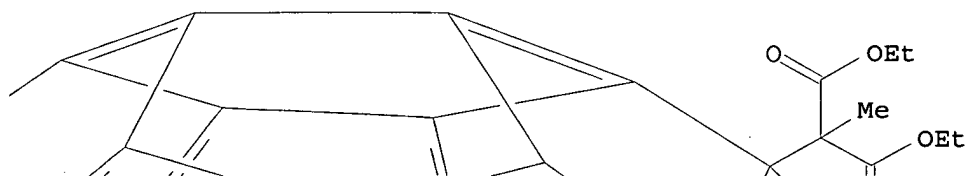


RN 910134-53-1 HCAPLUS  
 CN [5,6]Fullerene-C60-1h-1,23,28,33,38,60-hexaacetic acid,  
 $\alpha, \alpha', \alpha'', \alpha''', \alpha'''', \alpha'''''$ -  
 hexakis(ethoxycarbonyl)- $\alpha, \alpha', \alpha'', \alpha'''$ , .alpha  
 $''''', \alpha''''''$ -hexamethyl-, hexaethyl ester, radical ion(2-)  
 (9CI) (CA INDEX NAME)

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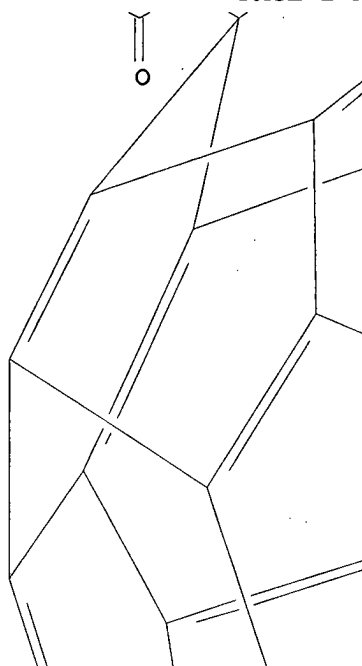


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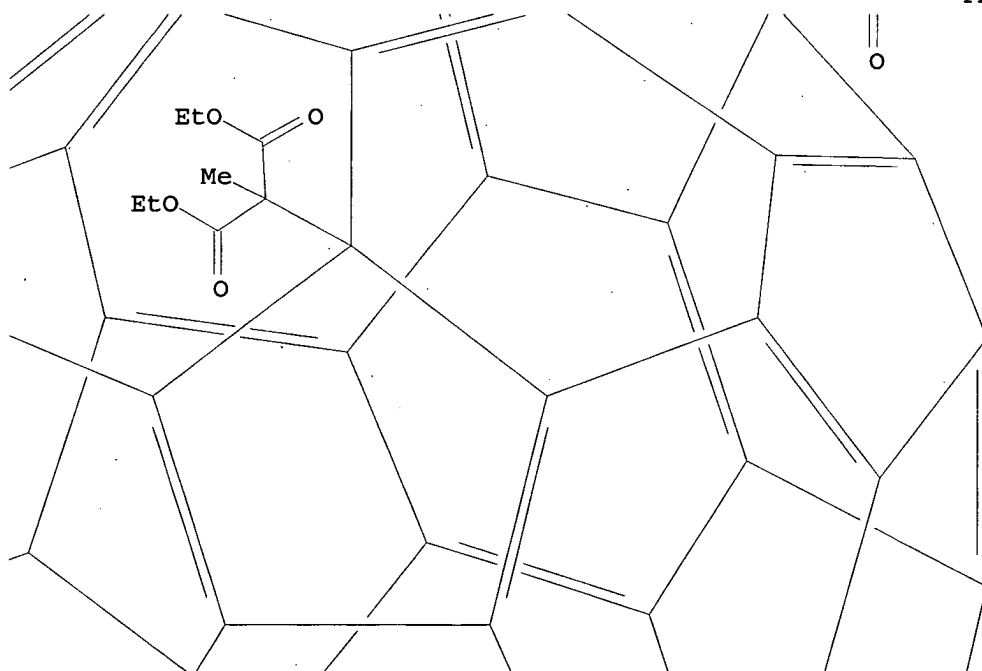




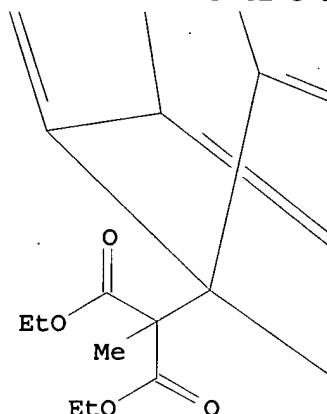
PAGE 2-A



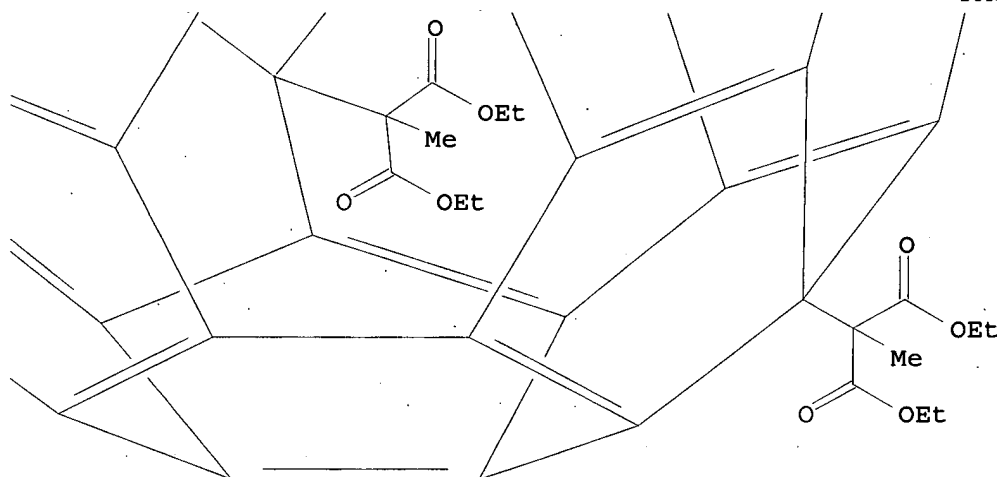
PAGE 2-B



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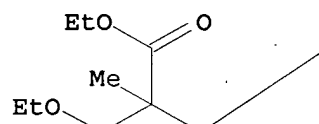
IT 910134-54-2

RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process)  
(electrochem. reductive formation and reduction potential in THF containing Bu<sub>4</sub>NPF<sub>6</sub>)

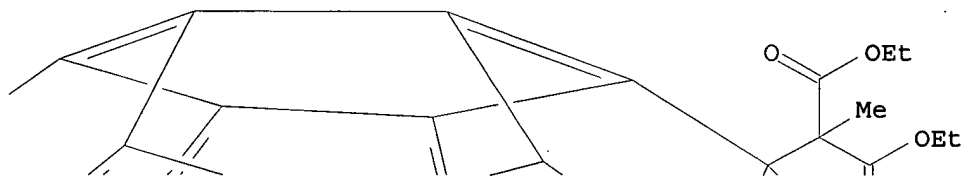
RN 910134-54-2 HCAPLUS

CN [5,6]Fullerene-C<sub>60</sub>-1h-1,23,28,33,38,60-hexaacetic acid,  
α,α',α'',α''',α''',α''''-  
hexakis(ethoxycarbonyl)-α,α',α'',α''',.alpha  
. ''',α''''-hexamethyl-, hexaethyl ester, radical ion(3-)  
(9CI) (CA INDEX NAME)

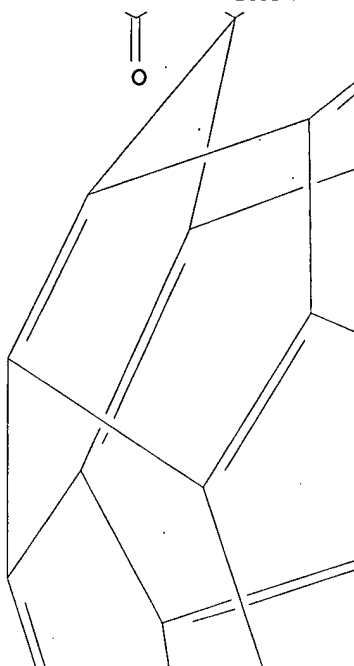
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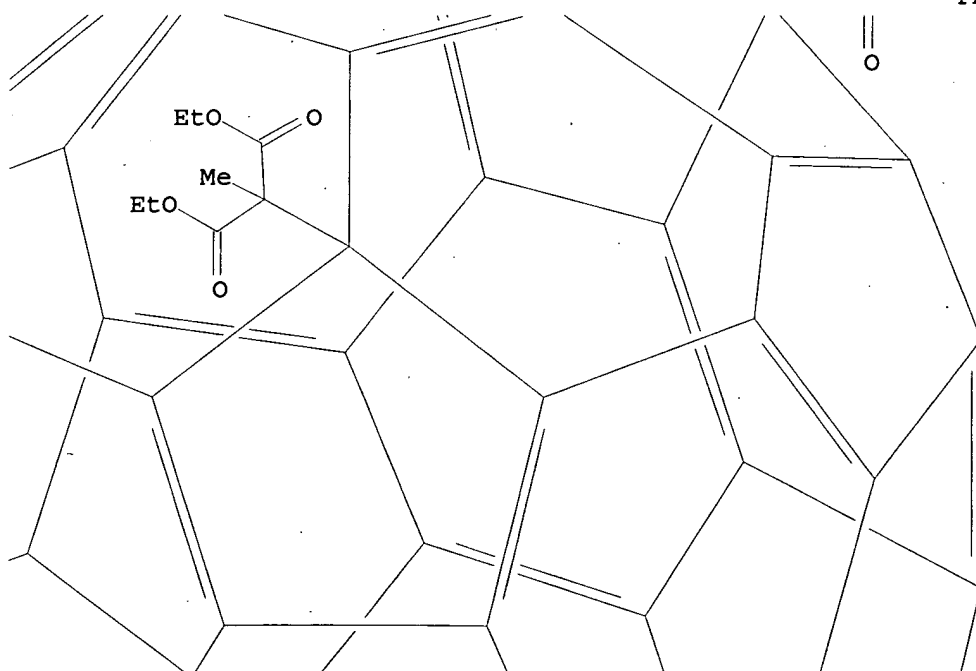
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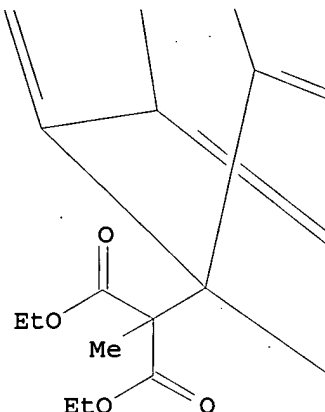
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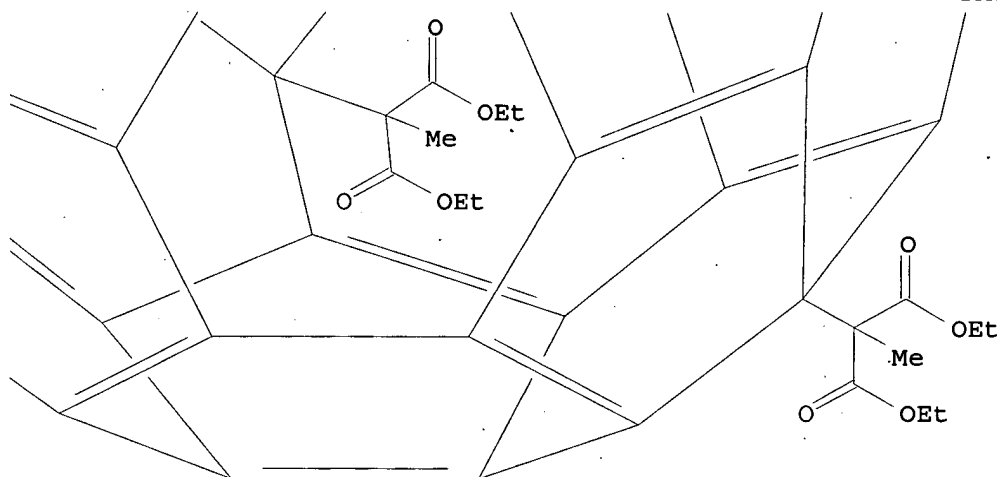
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- CC 72-2 (Electrochemistry)  
Section cross-reference(s): 22, 25
- IT 836649-08-2  
RL: PRP (Properties)  
(Schlegel diagram of)
- IT 836649-07-1  
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)  
(cyclic voltammetry in THF containing Bu<sub>4</sub>NPF<sub>6</sub> and low multielectron reduction potentials of emerald green [60]fullerenes)
- IT 910131-71-4 910134-53-1  
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)  
(electrochem. reductive formation and electrochem. reduction and reduction potential in THF containing Bu<sub>4</sub>NPF<sub>6</sub>)
- IT 910134-54-2  
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP

(Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process).  
(electrochem. reductive formation and reduction potential in THF containing Bu<sub>4</sub>NPF<sub>6</sub>)

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 4 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:748172 HCAPLUS

DOCUMENT NUMBER: 145:301696

TITLE: Unusual photophysical properties of emerald green [60]fullerene

AUTHOR(S): El-Khouly, Mohamed E.; Canteenwala, Taizoon; Araki, Yasuyuki; Ito, Osamu; Chiang, Long Y.

CORPORATE SOURCE: Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, 2-1-1 Katahira, Sendai, 980-8577, Japan

SOURCE: Chemistry Letters (2006), 35(7), 710-711  
CODEN: CMLTAG; ISSN: 0366-7022

PUBLISHER: Chemical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Near-IR absorptive emerald green [60]fullerene (EF-6MC2) is capable of highly light-harvesting mol. Photoinduced intermol. electron transfer between EF-6MC2 and several electron donors in benzonitrile led to observation of the optical absorption of (EF-6MC2).- at 1300 nm, the longest absorption wavelength among many [60]fullerenyl radical anions.

IT 836649-07-1D, derivs.

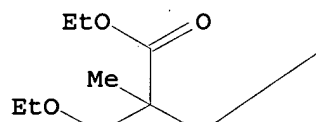
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(unusual photophys. properties of emerald green [60]fullerene)

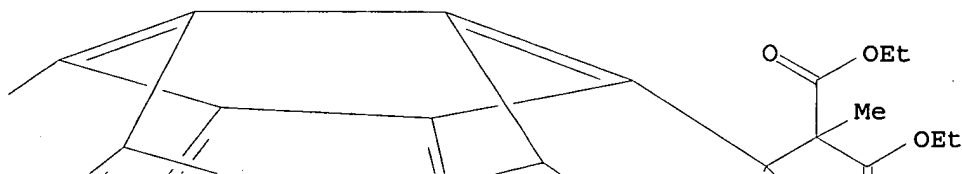
RN 836649-07-1 HCAPLUS

CN [5,6]Fullerene-C60-1h-1,23,28,33,38,60-hexaacetic acid,  
 $\alpha, \alpha', \alpha'', \alpha''', \alpha''''$ -  
hexakis(ethoxycarbonyl)- $\alpha, \alpha', \alpha'', \alpha'''$ , .alpha  
. ''',  $\alpha''''$ -hexamethyl-, hexaethyl ester (9CI) (CA INDEX  
NAME)

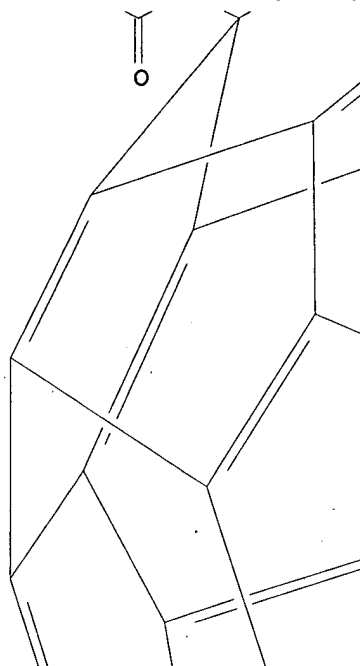
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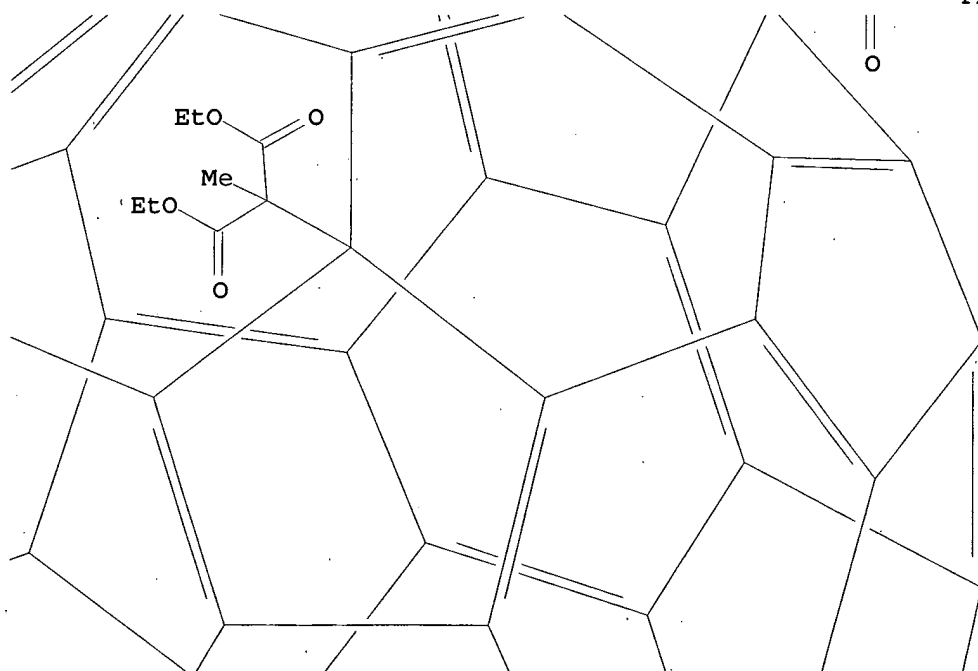
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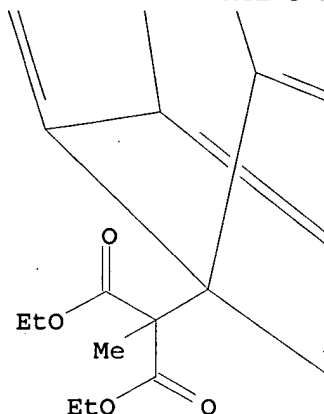


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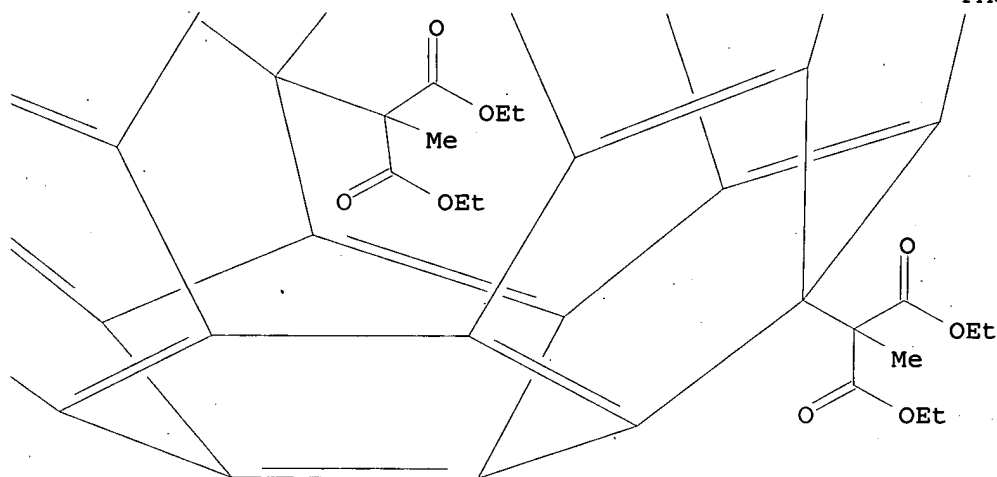




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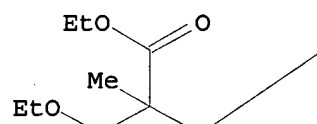
IT 836649-07-1

RL: PEP (Physical, engineering or chemical process); PRP  
(Properties); PYP (Physical process); PROC (Process)  
(unusual photophys. properties of emerald green [60]fullerene)

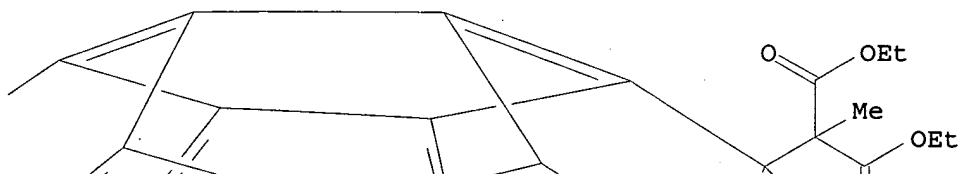
RN 836649-07-1 HCAPLUS

CN [5,6]Fullerene-C60-Ih-1,23,28,33,38,60-hexaacetic acid,  
 $\alpha, \alpha', \alpha'', \alpha''', \alpha''''$ -  
hexakis(ethoxycarbonyl)- $\alpha, \alpha', \alpha'', \alpha'''$ , .alpha  
. ''',  $\alpha''''$ -hexamethyl-, hexaethyl ester (9CI) (CA INDEX  
NAME)

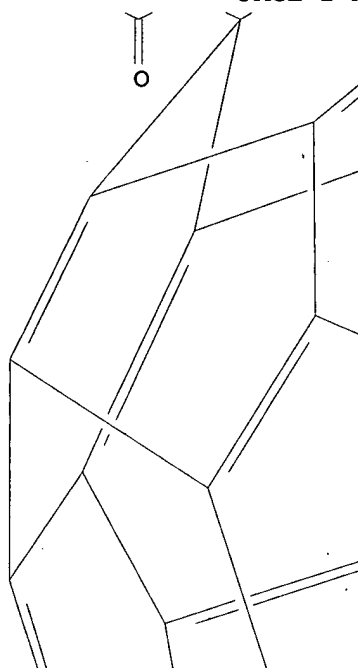
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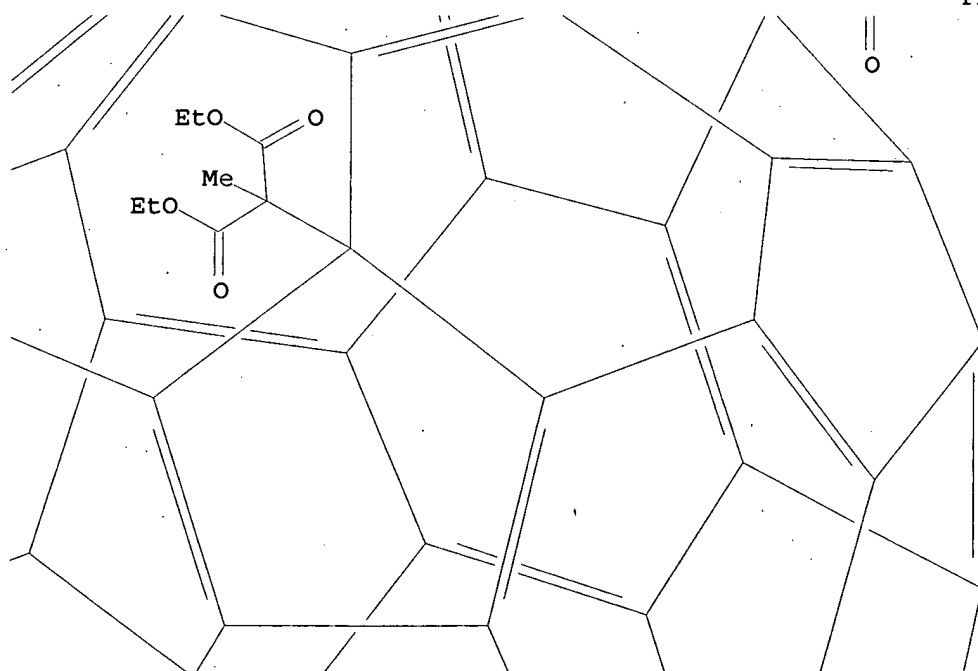
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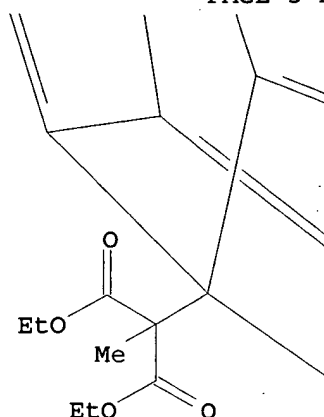
PAGE 2-A



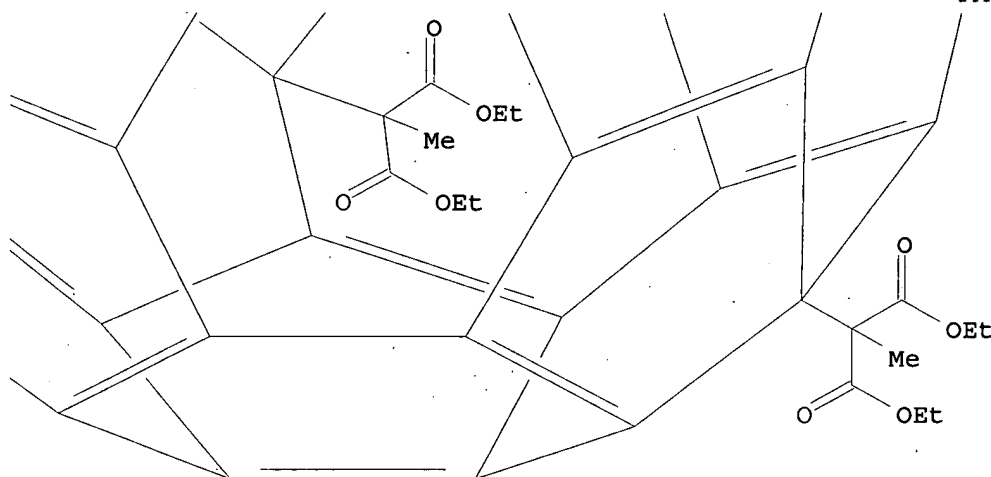
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CC 73-4 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)  
 IT 836649-07-1D, derivs.  
 RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)  
 (unusual photophys. properties of emerald green [60]fullerene)  
 IT 996-70-3, Tetrakis(dimethylamino)ethylene 836649-07-1  
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)  
 (unusual photophys. properties of emerald green [60]fullerene)  
 REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 5 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2006:478699 HCAPLUS  
 DOCUMENT NUMBER: 145:154692  
 TITLE: Electronic Structure and Spectroscopic Studies of D3d-C60Cl30, a Chlorofullerene with a

[18]Trannulene Ring, and Its Relation to Other  
[18]Trannulenes

AUTHOR(S): Popov, Alexey A.; Senyavin, Vladimir M.;  
Trojanov, Sergey I.

CORPORATE SOURCE: Chemistry Department, Moscow State University,  
Moscow, 119992, Russia

SOURCE: Journal of Physical Chemistry A (2006), 110(23),  
7414-7421  
CODEN: JPCAFH; ISSN: 1089-5639

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

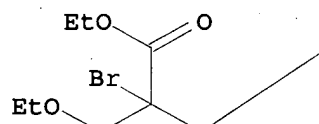
AB Detailed spectroscopic characterization of D3d-C60Cl30, including  
IR, Raman, UV-visible absorption, and fluorescence spectra, is  
presented for the 1st time. Assignment of the vibrational spectra  
is proposed from d. functional theory computations. Electronic  
structure and excitations of C60Cl30 and other [18]trannulenes are  
studied theor. using time-dependent d. functional theory and  
time-dependent Hartree-Fock approximation Assignment of the low-energy  
part of electronic spectra of C60-based [18]trannulenes is given and  
importance of the interactions between trannulene moiety and  
remaining  $\pi$ -subsystems in these mols. is established.

IT 899835-58-6  
RL: PRP (Properties)  
(electronic structure and spectroscopic studies of D3d-C60Cl30,  
chlorofullerene with [18]Trannulene ring and relation to other  
[18]Trannulenes)

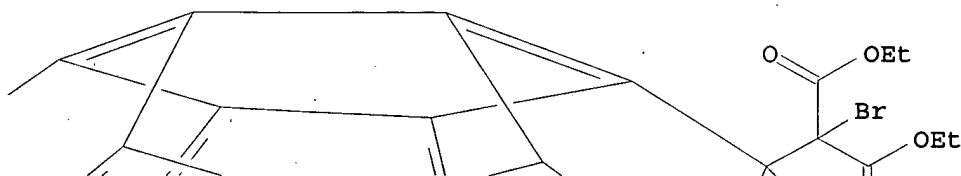
RN 899835-58-6 HCAPLUS

CN [5,6]Fullerene-C60-1h-1,23,28,33,38,60-hexaacetic acid,  
 $\alpha, \alpha', \alpha'', \alpha''', \alpha'''', \alpha'''''$ -  
hexabromo- $\alpha, \alpha', \alpha'', \alpha''', \alpha'''', \alpha'''''$ -  
''''-hexakis(ethoxycarbonyl)-, hexaethyl ester (9CI) (CA INDEX  
NAME)

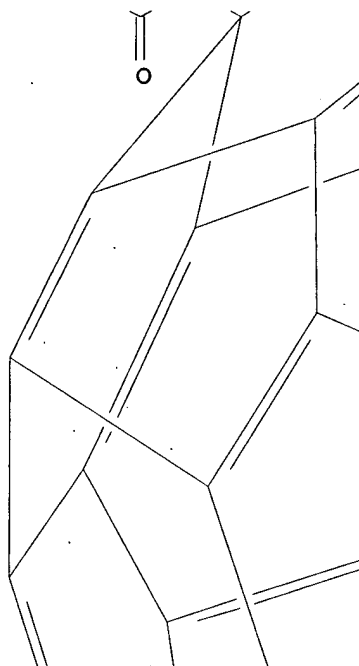
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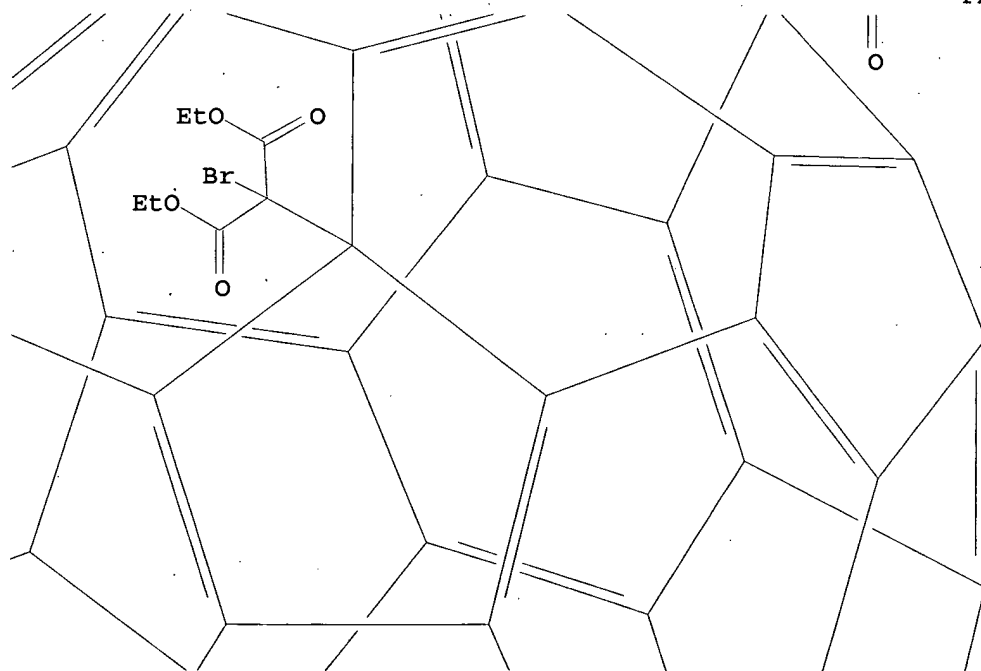
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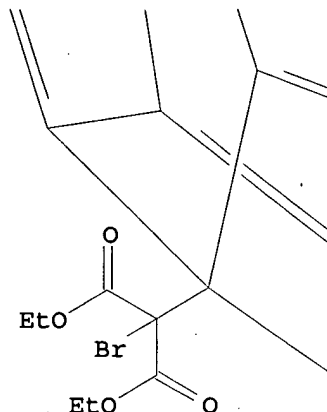
PAGE 2-A



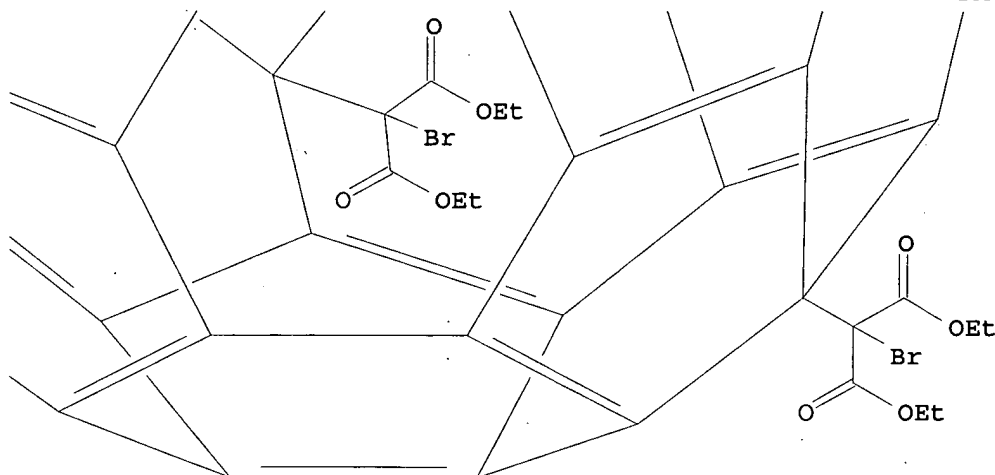
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CC 73-4 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)

IT 156-80-9D, Malonate, derivs. 90762-52-0, [18]Trannulene  
 99685-96-8, C60 Fullerene 167696-95-9 185912-87-2 405910-77-2  
 405910-83-0 405910-87-4 475975-85-0 831227-44-2 847229-48-5  
 899835-56-4 899835-57-5 **899835-58-6** 899835-59-7  
 899835-60-0 899835-61-1 899835-62-2 899835-63-3

RL: PRP (Properties)

(electronic structure and spectroscopic studies of D3d-C60C130, chlorofullerene with [18]Trannulene ring and relation to other [18]Trannulenes)

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 6 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:342064 HCAPLUS

DOCUMENT NUMBER: 145:7835

TITLE: Synthesis and Characterization of a Bisadduct of



AUTHOR(S): La@C82  
Feng, Lai; Tsuchiya, Takahiro; Wakahara,  
Takatsugu; Nakahodo, Tsukasa; Piao, Qiuyue;  
Maeda, Yutaka; Akasaka, Takeshi; Kato,  
Tatsuhisa; Yoza, Kenji; Horn, Ernst; Mizorogi,  
Naomi; Nagase, Shigeru

CORPORATE SOURCE: Center for Tsukuba Advanced Research Alliance,  
University of Tsukuba, Tsukuba, 305-8577, Japan

SOURCE: Journal of the American Chemical Society (2006),  
128(18), 5990-5991  
CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:7835

AB A bisadduct of La@C82(C2v), La@C82[CH(COOEt)2]2, was synthesized in  
a good yield by a Bingel-Hirsch reaction. Its structure was  
well-defined by x-ray crystallog. anal. A pair of enantiomers of  
the adduct form a dimer in the single crystal. The bisadduct was  
further characterized by its ESR and UV-visible-NIR spectra and its  
redox potentials were measured by differential pulse voltammetry  
(DPV).

IT 888318-48-7P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP  
(Preparation)  
(preparation and crystal structure of dimer of a Bingel-Hirsch  
bisadduct of lanthanum endohedral fullerene-C82)

RN 888318-48-7 HCAPLUS

CN 48,48' (1H,1'H)-Bi[5,6]fullerene-C82-C2v-1,1'-diyl,  
67,67',70,70'-tetrakis[2-ethoxy-1-(ethoxycarbonyl)-2-oxoethyl]-,  
radical ion(6-), dilanthanum(3+), compd. with hexane (1:2) (9CI)  
(CA INDEX NAME)

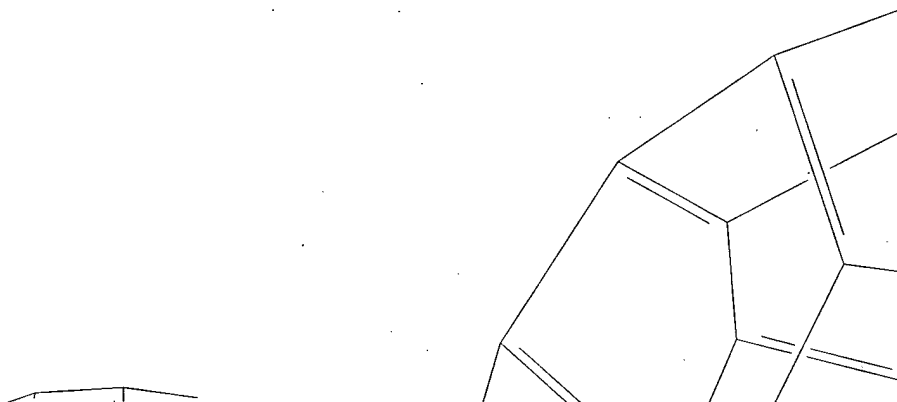
CM 1

CRN 888212-74-6

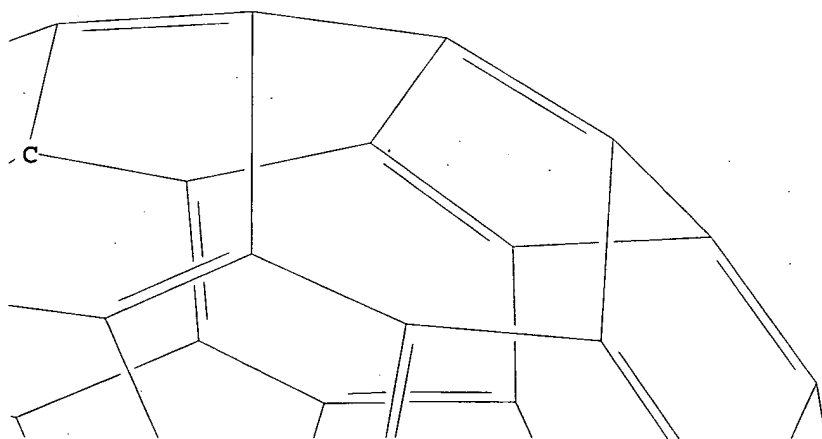
CMF C192 H44 O16

CCI RIS

PAGE 1-B



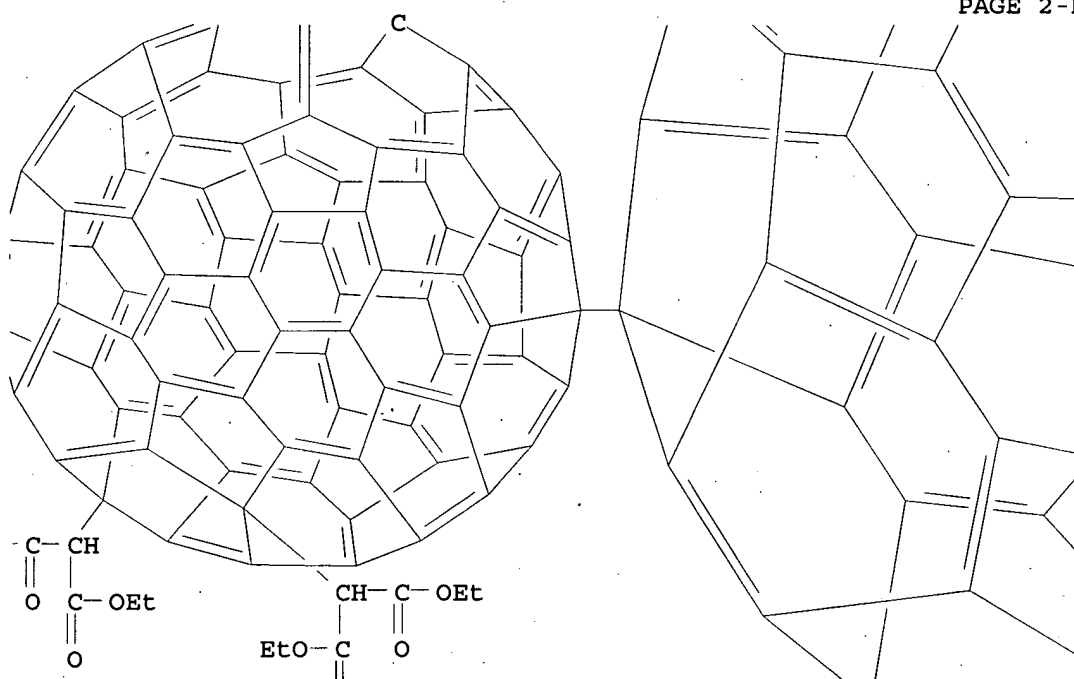
PAGE 1-C



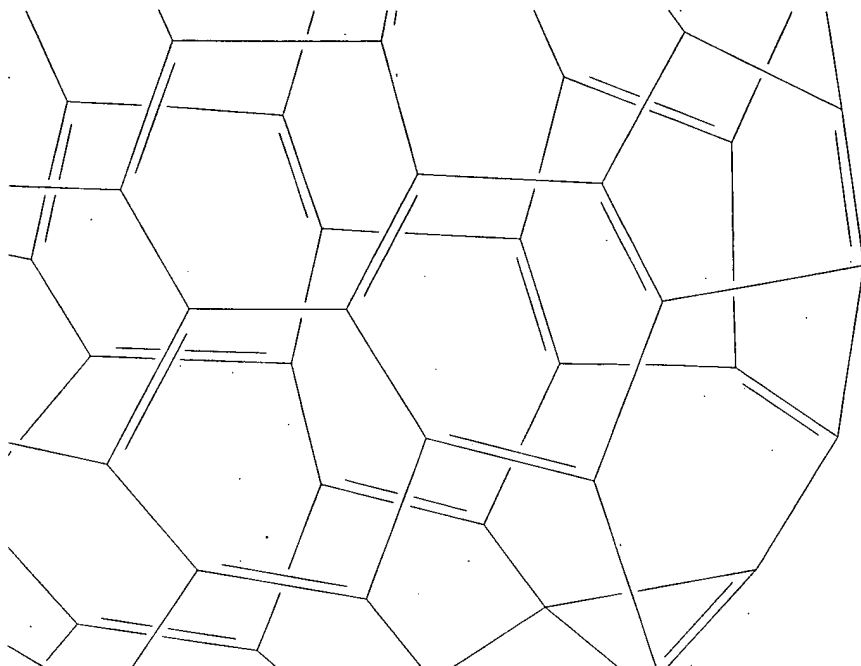
PAGE 2-A

EtO-

PAGE 2-B

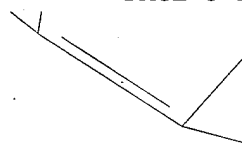


PAGE 2-C

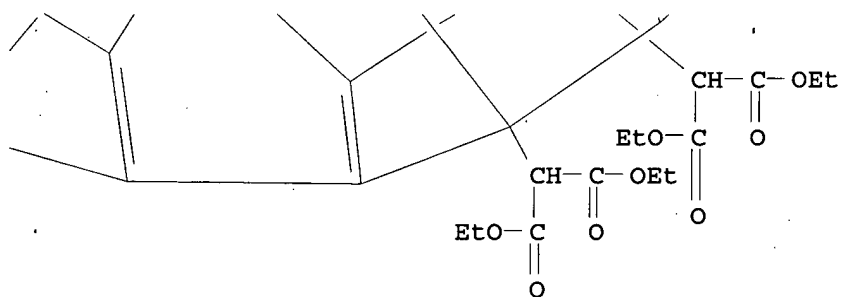


PAGE 3-B

O



PAGE 3-C



CM 2

CRN 110-54-3  
CMF C6 H14

Me-(CH<sub>2</sub>)<sub>4</sub>-Me

IT 888069-01-0P

RL: PRP (Properties); SPN (Synthetic preparation); PREP  
(Preparation)

(preparation and mol. structure of dimer of a Bingel-Hirsch bisadduct  
of lanthanum endohedral fullerene-C82)

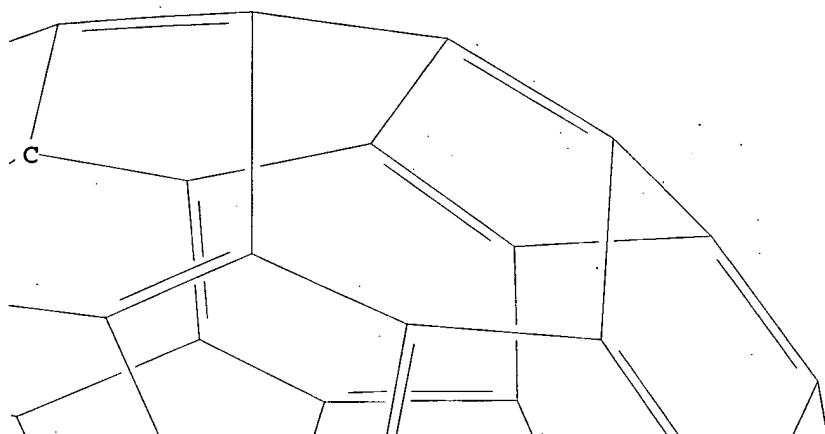
RN 888069-01-0 HCAPLUS

CN 48,48' (1H,1'H)-Bi[5,6]fullerene-C82-C2v-1,1'-diyl,  
67,67',70,70'-tetrakis[2-ethoxy-1-(ethoxycarbonyl)-2-oxoethyl]-,  
radical ion(6-), dilanthanum(3+) (9CI) (CA INDEX NAME)

PAGE 1-B



PAGE 1-C

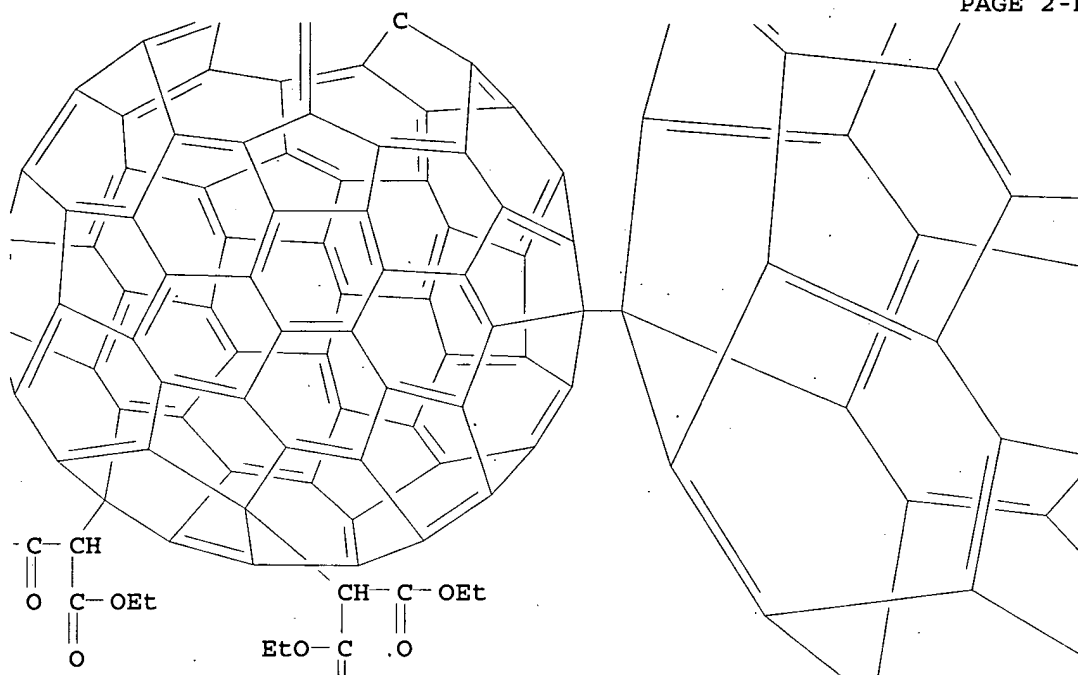


PAGE 2-A

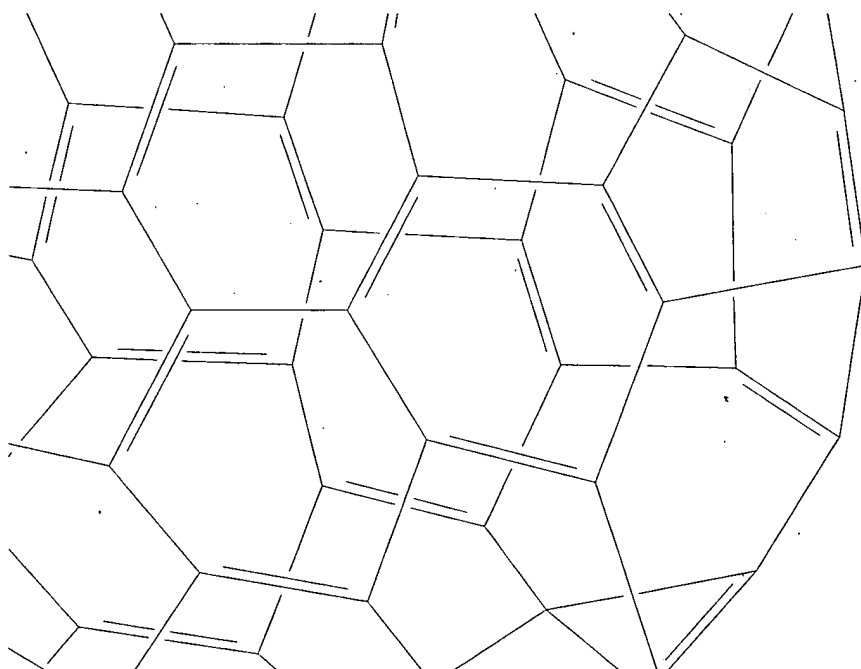


EtO-

PAGE 2-B



PAGE 2-C



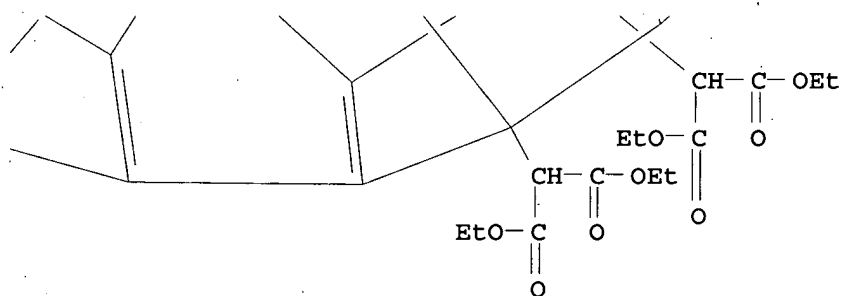
PAGE 3-A

●2 La(III) <sup>3+</sup>

PAGE 3-B

O

PAGE 3-C



IT 888318-46-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of a Bingel-Hirsch bisadduct of lanthanum endohedral  
 fullerene-C82)

RN 888318-46-5 HCAPLUS

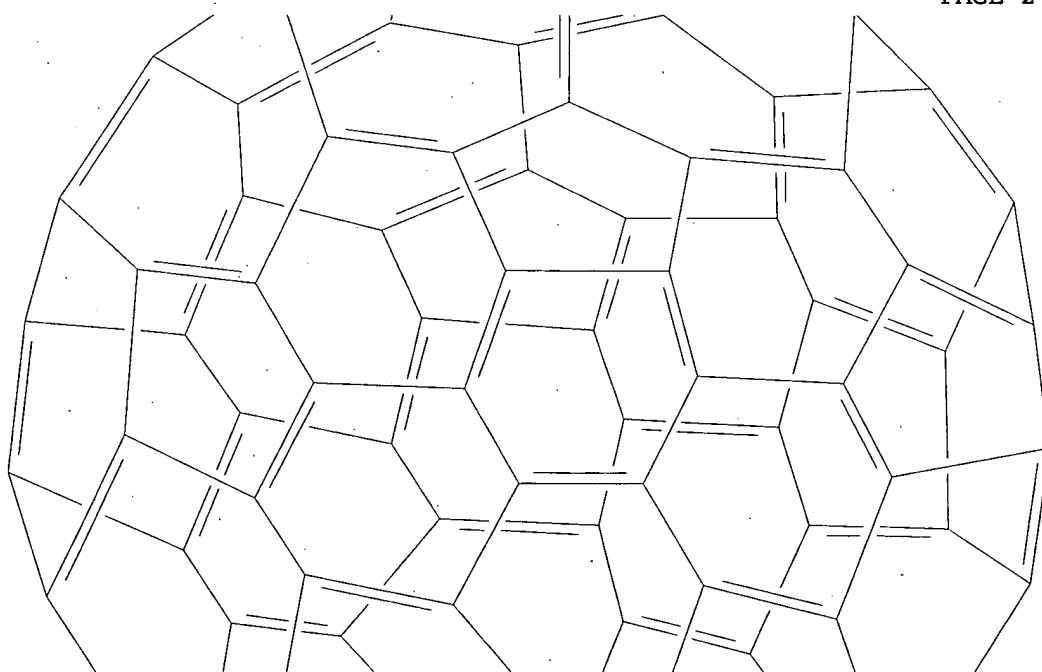
CN [5,6]Fullerene-C82-C2v-67,70-diacetic acid,  $\alpha,\alpha'$ -  
 bis(ethoxycarbonyl)-, radical ion(4-), lanthanum(3+) (9CI) (CA  
 INDEX NAME)



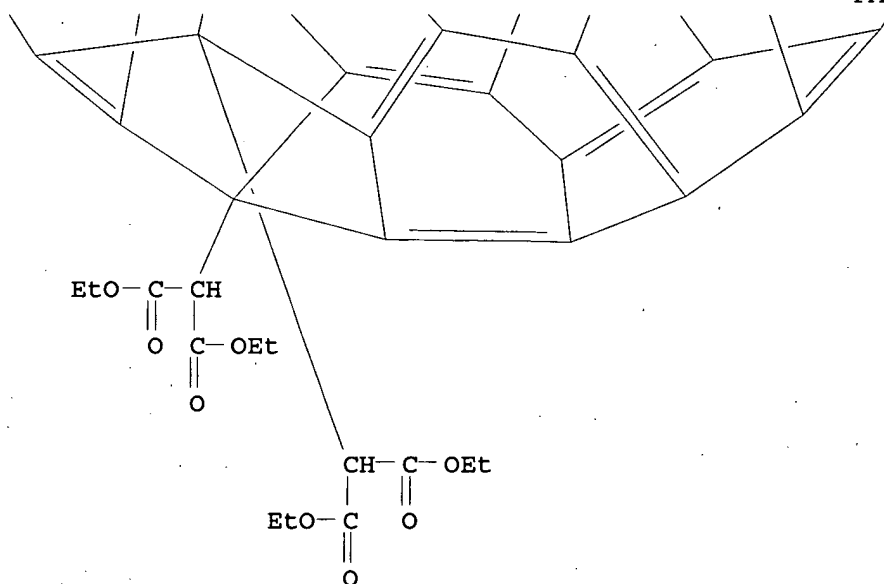
PAGE 1-A



PAGE 2-A



PAGE 3-A



PAGE 4-A

● La(III) 3+

IT 888069-00-9P

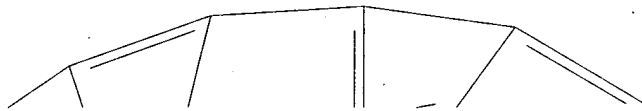
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation);  
 PREP (Preparation); RACT (Reactant or reagent)

(preparation, ESR and UV-visible-NIR spectra, redox potentials and  
 dimerization upon crystallization of a Bingel-Hirsch bisadduct of  
 lanthanum endohedral fullerene-C82)

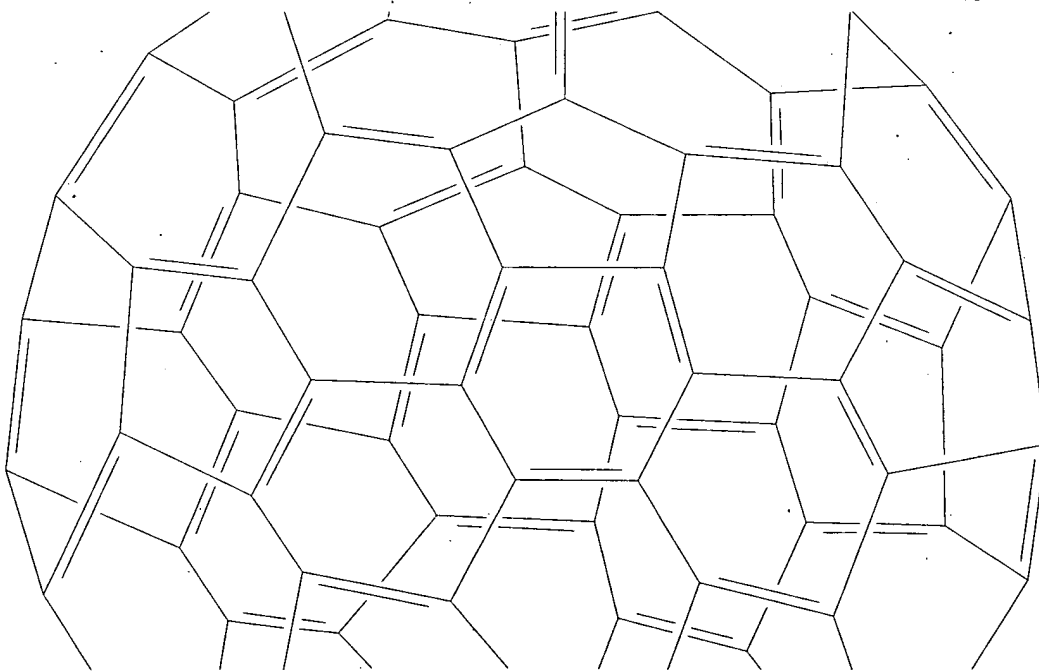
RN 888069-00-9 HCAPLUS

CN [5,6]Fullerene-C82-C2v-67,70-diacetic acid,  $\alpha,\alpha'$ -  
 bis(ethoxycarbonyl)-, radical ion(3-), lanthanum(3+) (9CI) (CA  
 INDEX NAME)

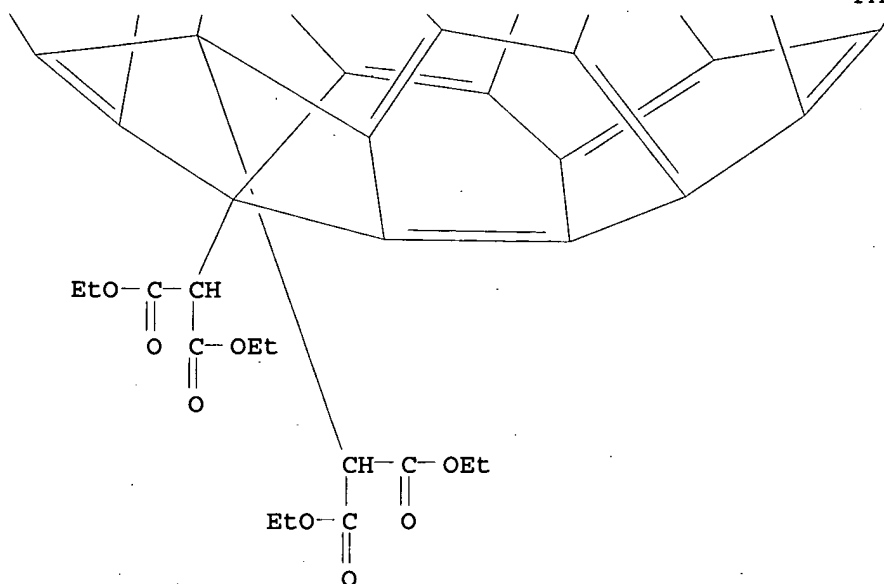
PAGE 1-A



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PAGE 3-A



PAGE 4-A

● La(III) 3+

- CC 25-29 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
Section cross-reference(s): 75, 78
- IT 888318-48-7P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal structure of dimer of a Bingel-Hirsch bisadduct of lanthanum endohedral fullerene-C82)
- IT 888069-01-0P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and mol. structure of dimer of a Bingel-Hirsch bisadduct of lanthanum endohedral fullerene-C82)
- IT 888318-46-5P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of a Bingel-Hirsch bisadduct of lanthanum endohedral fullerene-C82)
- IT 888069-00-9P  
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation, ESR and UV-visible-NIR spectra, redox potentials and dimerization upon crystallization of a Bingel-Hirsch bisadduct of lanthanum endohedral fullerene-C82)
- REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 7 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2005:1085982 HCAPLUS  
DOCUMENT NUMBER: 144:43080

TITLE: Fluorinated Fullerenes: Sources of  
Donor-Acceptor Dyads with [18]Trannulene  
Acceptors for Energy- and Electron-Transfer  
Reactions

AUTHOR(S): Guldi, Dirk M.; Marcaccio, Massimo; Paolucci,  
Francesco; Paolucci, Demis; Ramey, Jeff; Taylor,  
Roger; Burley, Glenn A.

CORPORATE SOURCE: Institute for Physical and Theoretical  
Chemistry, Universitaet Erlangen, Erlangen,  
91058, Germany

SOURCE: Journal of Physical Chemistry A (2005), 109(43),  
9723-9730  
CODEN: JPCAFH; ISSN: 1089-5639

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

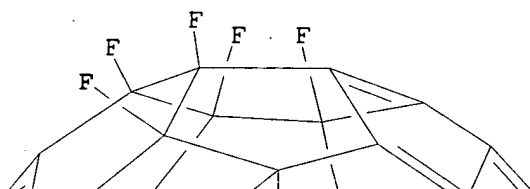
AB Fine-tuned control over the donor strength in a series of  
trannulenes-based donor-acceptor ensembles is used to alter the  
deactivation path of the photoexcited-state chromophore and to  
modulate the rates of intramol. electron transfer. For the first  
time, a detailed anal. of emission spectra, time-dependent  
spectroscopic measurements, and electrochem. prove spectroscopically  
and kinetically that trannulenes can serve, in a manner similar to  
C60 and C60 monoadducts, as both electron and also as energy  
acceptor in donor-acceptor ensembles, producing widely different  
electron-transfer regimes. This investigation also shows that the  
integration of trannulenes, as a versatile electron-acceptor  
building block, consistently produces charge recombination in the  
inverted Marcus region.

IT 658065-06-6 681846-12-8 681846-23-1  
RL: PEP (Physical, engineering or chemical process); PRP  
(Properties); PYP (Physical process); PROC (Process)  
(electrochem. and photophys. properties of trannulene based  
donor-acceptor dyad ensembles)

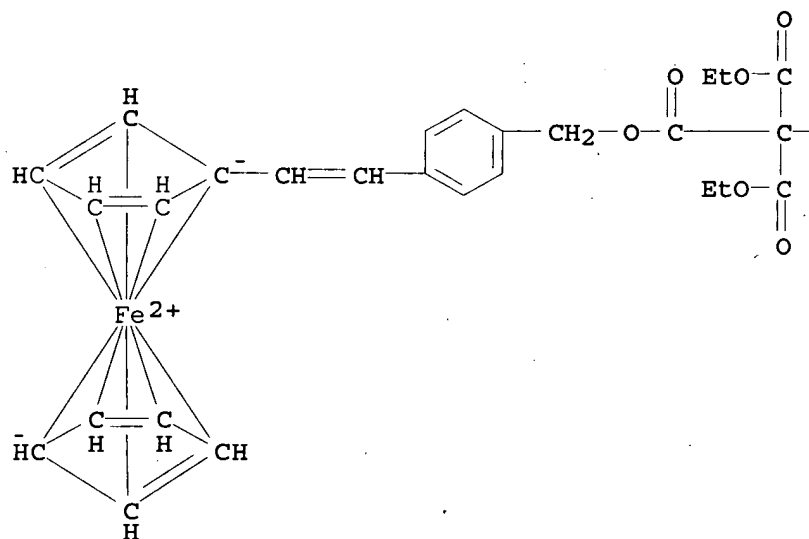
RN 658065-06-6 HCAPLUS

CN Ferrocene, 1,1',1''',1''''-[(23,24,25,26,27,28,41,42,47,48,49,55,56,59,6  
0-pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
tetradecahydro[5,6]fullerene-C60-Ih-1,33,38(23H)-triyl)tris[[2,2-  
bis(ethoxycarbonyl)-1-oxo-2,1-ethanediyl]oxymethylene-4,1-phenylene-  
2,1-ethenediyl]]tris- (9CI) (CA INDEX NAME)

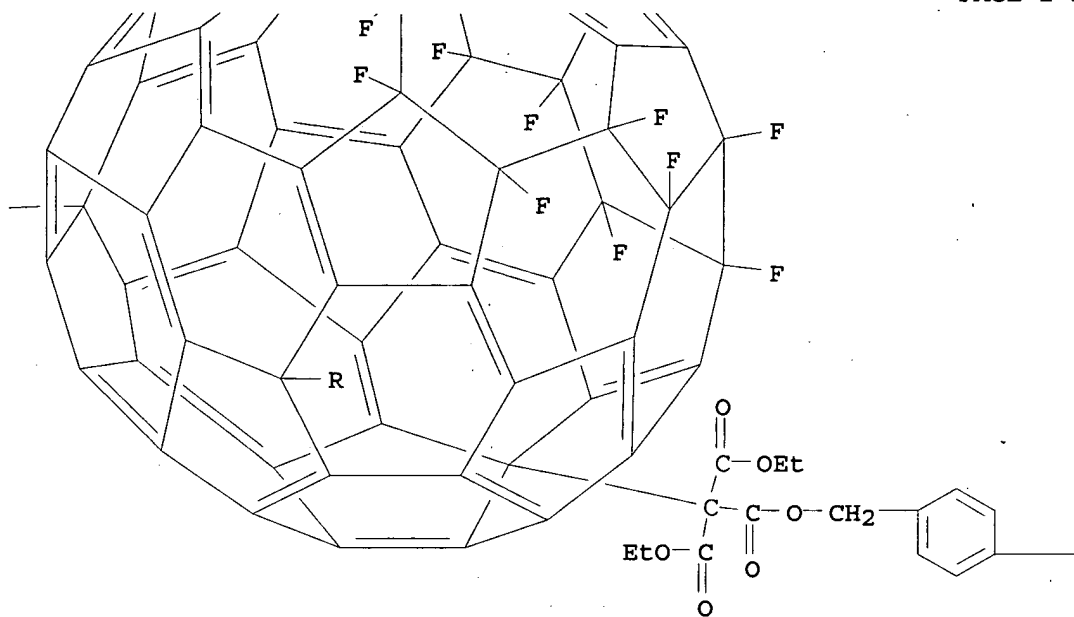
PAGE 1-B



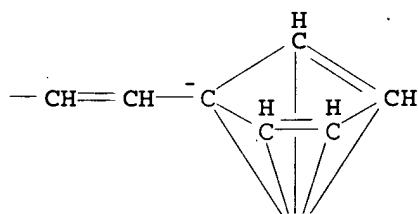
PAGE 2-A



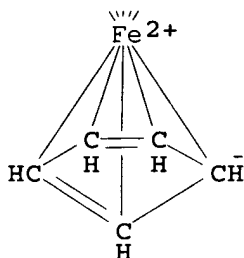
PAGE 2-B



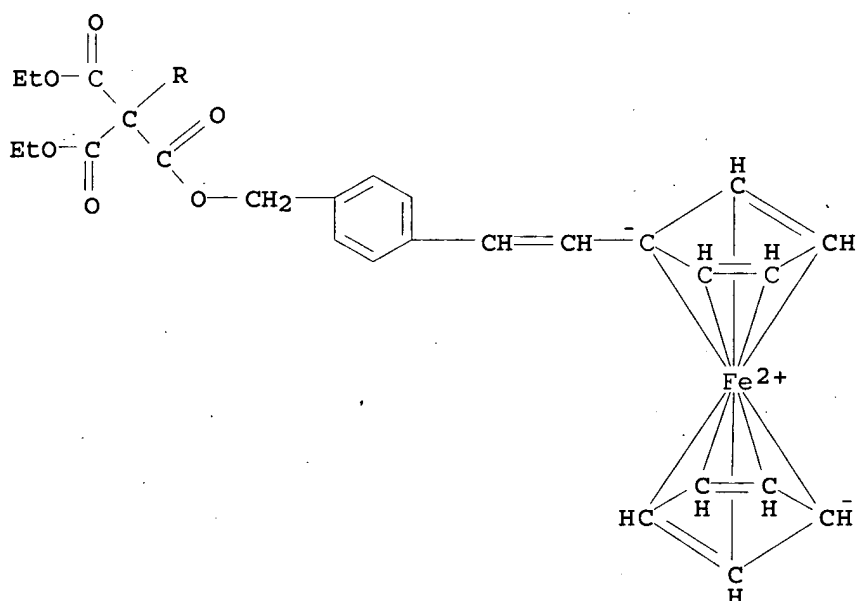
PAGE 2-C



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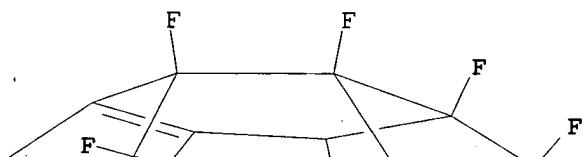
PAGE 4-A



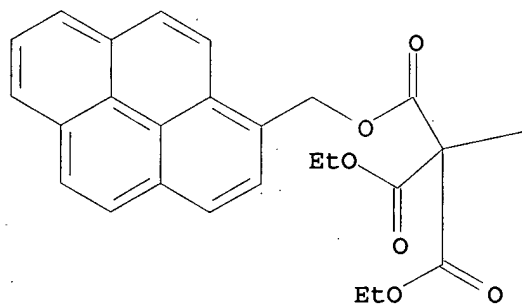
RN 681846-12-8 HCAPLUS  
 CN [5,6]Fullerene-C60-Ih-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha,\alpha',\alpha',\alpha'',\alpha''$ -  
 hexakis(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 tetradecahydro-, tris(1-pyrenylmethyl) ester (9CI) (CA INDEX NAME)



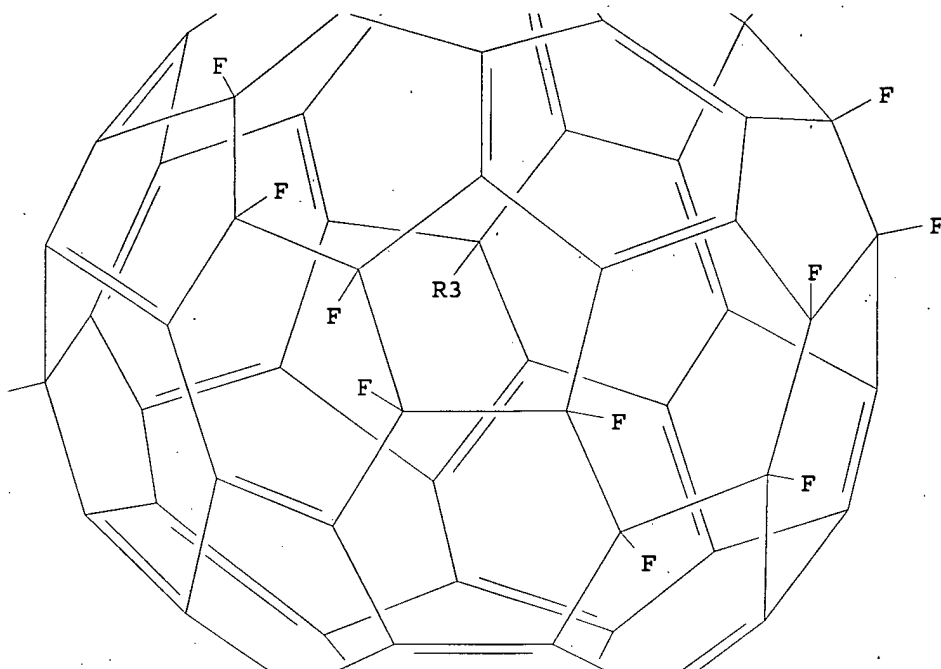
PAGE 1-B



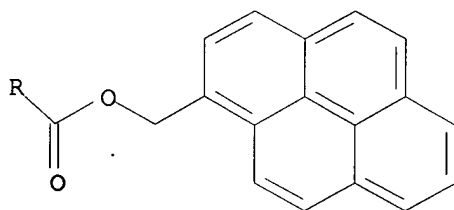
PAGE 2-A



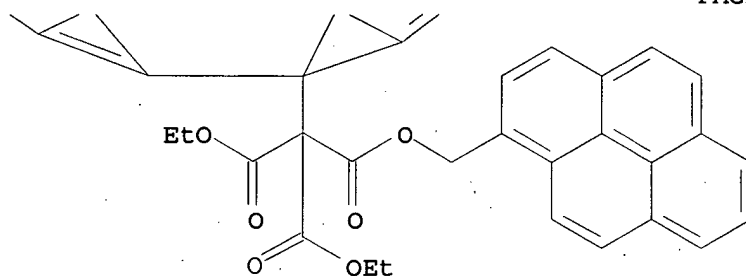
PAGE 2-B



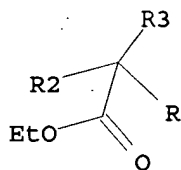
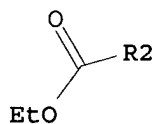
PAGE 3-A



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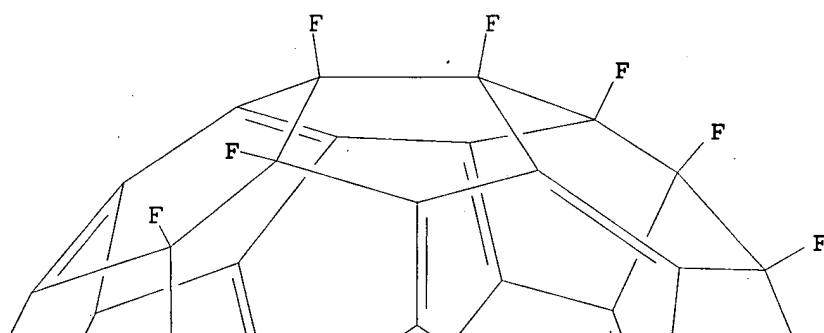


PAGE 4-A

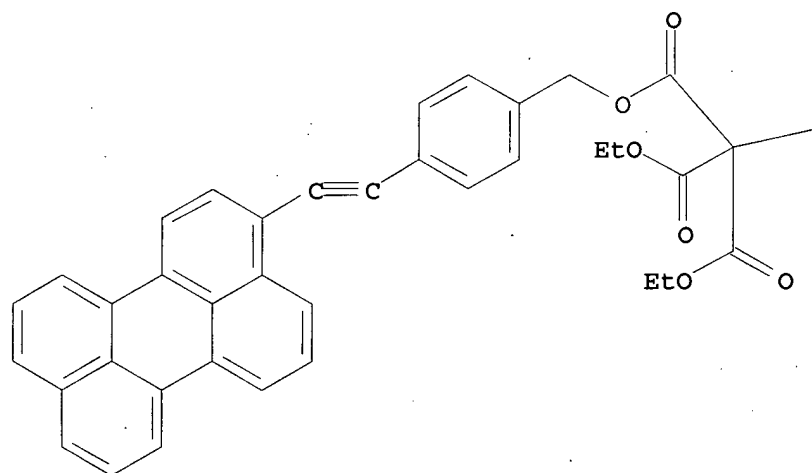


RN 681846-23-1 HCAPLUS  
 CN [5,6]Fullerene-C60-1h-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha,\alpha',\alpha',\alpha'',\alpha''$ -  
 hexakis(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 tetradecahydro-, tris[[4-(3-perylenylethynyl)phenyl]methyl] ester  
 (9CI) (CA INDEX NAME)

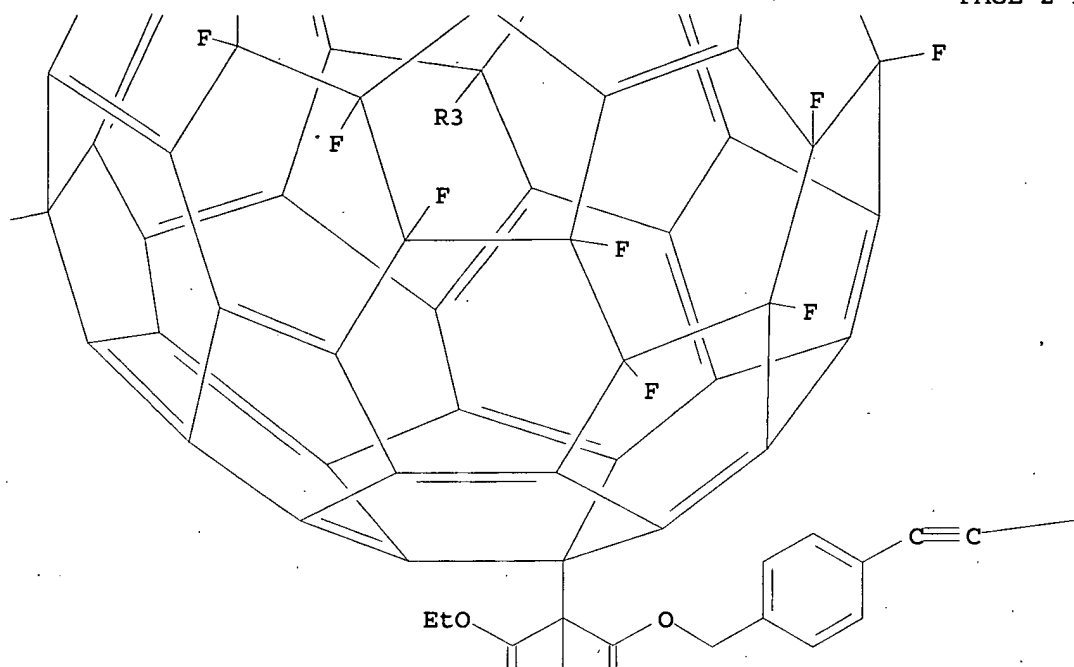
PAGE 1-B



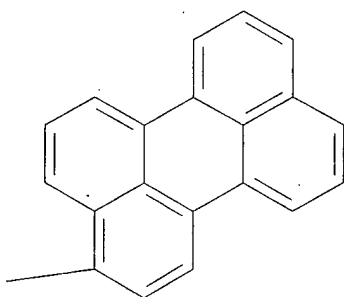
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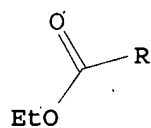
PAGE 2-B



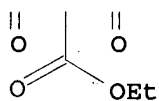
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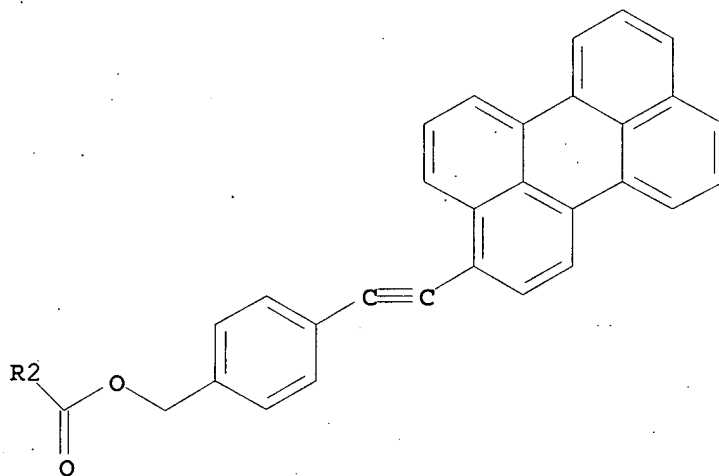
PAGE 3-A



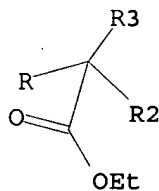
PAGE 3-B



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PAGE 5-A



IT 658065-04-4

RL: PEP (Physical, engineering or chemical process); PRP

(Properties); PYP (Physical process); PROC (Process)  
(reference; electrochem. and photophys. properties of trannulene based  
donor-acceptor dyad ensembles)

RN 658065-04-4 HCAPLUS

CN [5,6]Fullerene-C60-Ih-1,33,38(23H)-triacetic acid,

 $\alpha, \alpha, \alpha', \alpha', \alpha'', \alpha'' -$ 

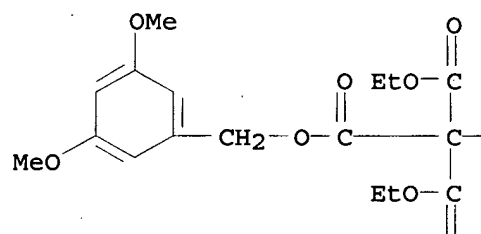
hexakis(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-

pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-

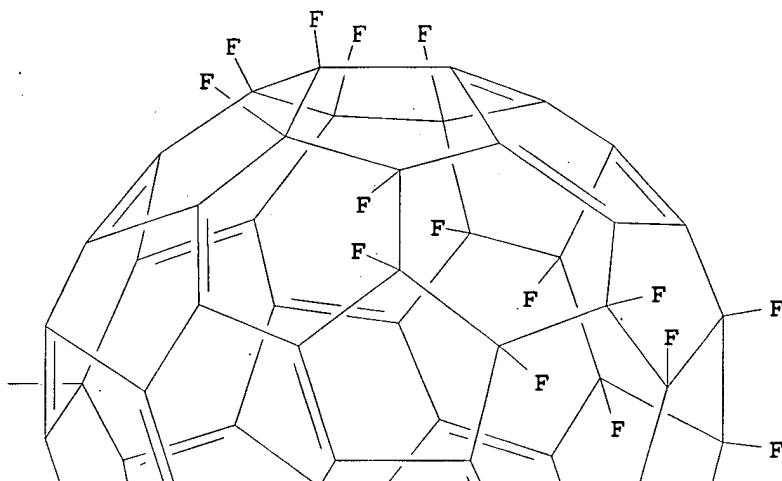
tetradecahydro-, tris[(3,5-dimethylphenyl)methyl] ester (9CI) (CA

INDEX NAME)

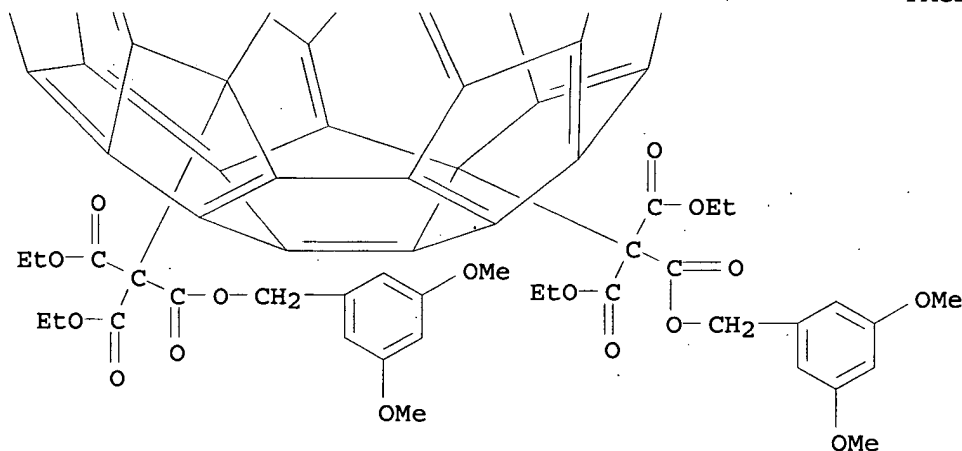
PAGE 1-A



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PAGE 2-A  
O

PAGE 2-B

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and  
Other Reprographic Processes)

Section cross-reference(s): 72, 73

IT 658065-06-6 681846-12-8 681846-23-1

RL: PEP (Physical, engineering or chemical process); PRP



(Properties); PYP (Physical process); PROC (Process)  
(electrochem. and photophys. properties of trannulene based  
donor-acceptor dyad ensembles)

IT 658065-04-4

RL: PEP (Physical, engineering or chemical process); PRP  
(Properties); PYP (Physical process); PROC (Process)  
(reference; electrochem. and photophys. properties of trannulene based  
donor-acceptor dyad ensembles)

REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE  
FOR THIS RECORD. ALL CITATIONS AVAILABLE  
IN THE RE FORMAT

L12 ANSWER 8 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:1068088 HCAPLUS

DOCUMENT NUMBER: 142:206717

TITLE: Intense Near-Infrared Optical Absorbing Emerald  
Green [60]Fullerenes

AUTHOR(S): Canteenwala, Taizoon; Padmawar, Prashant A.;  
Chiang, Long Y.

CORPORATE SOURCE: Department of Chemistry, Institute of  
Nanoscience and Engineering Technology,  
University of Massachusetts, Lowell, MA, 01854,  
USA

SOURCE: Journal of the American Chemical Society (2005),  
127(1), 26-27

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Synthesis of emerald green fullerenes (EF) C<sub>60</sub>[CMe(CO<sub>2</sub>Et)<sub>2</sub>]<sub>6</sub> and  
C<sub>60</sub>[CMe(CO<sub>2</sub>-t-Bu)<sub>2</sub>]<sub>6</sub> was performed by using hexaanionic C<sub>60</sub>  
intermediate (C<sub>60</sub>-6) as a reagent in 1-pot reaction for attaching  
six alkyl ester addends on one C<sub>60</sub> cage. These EF compds. exhibit  
intense optical absorption over 600-940 nm, the longest optical  
absorption of the C<sub>60</sub> cage among many [60]fullerene derivs.  
synthesized.

IT 836649-07-1P 836649-08-2P

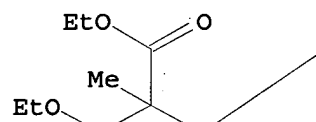
RL: PRP (Properties); SPN (Synthetic preparation); PREP  
(Preparation)

(intense near-IR optical absorbing emerald green [60]Fullerenes)

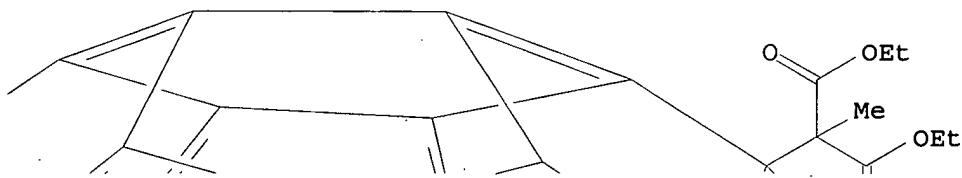
RN 836649-07-1 HCAPLUS

CN [5,6]Fullerene-C<sub>60</sub>-1h-1,23,28,33,38,60-hexaacetic acid,  
α,α',α'',α''',α''''',α''''''-  
hexakis(ethoxycarbonyl)-α,α',α'',α''',.alpha  
. ''''',α''''''-hexamethyl-, hexaethyl ester (9CI) (CA INDEX  
NAME)

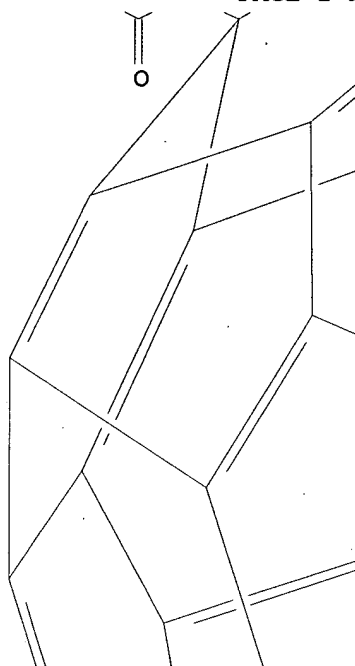
PAGE 1-A



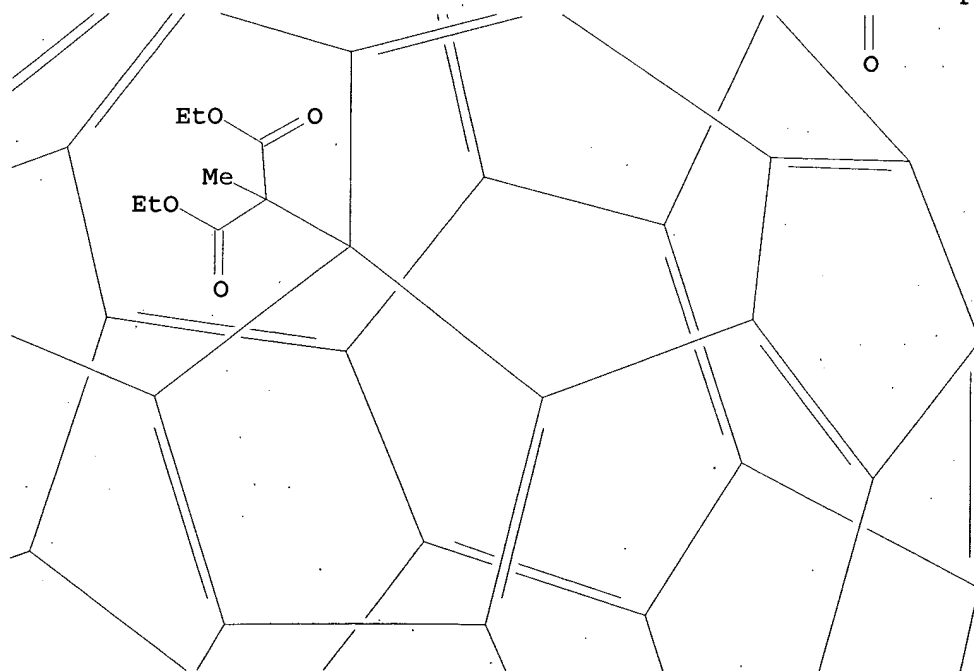
PAGE 1-B



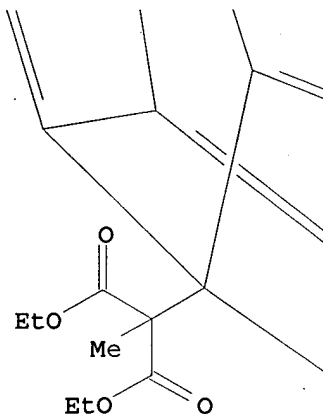
PAGE 2-A



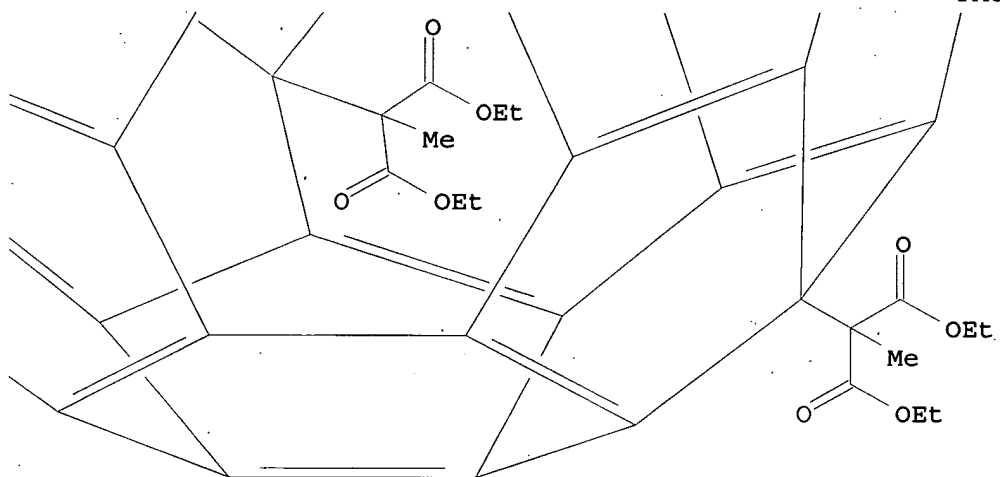
PAGE 2-B



PAGE 3-A

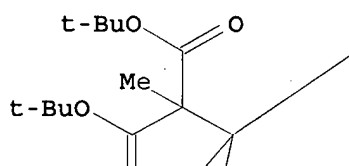


PAGE 3-B

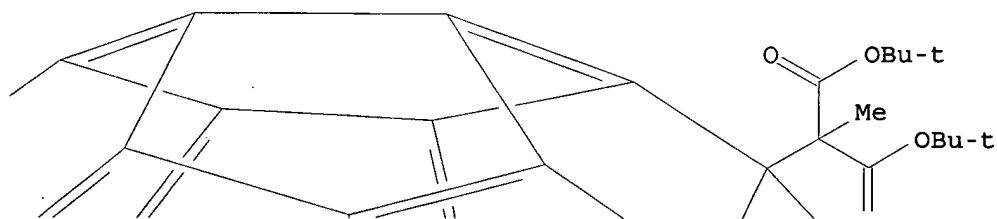


RN 836649-08-2 HCAPLUS  
 CN [5,6]Fullerene-C60-1h-1,23,28,33,38,60-hexaacetic acid,  
 $\alpha$ 1, $\alpha$ 23, $\alpha$ 28, $\alpha$ 33, $\alpha$ 38, $\alpha$ 60-  
 hexakis[(1,1-dimethylethoxy)carbonyl]- $\alpha$ 1, $\alpha$ 23, $\alpha$ 28,  
 $\alpha$ 33, $\alpha$ 38, $\alpha$ 60-hexamethyl-, 1,23,28,33,38,60-  
 hexakis(1,1-dimethylethyl) ester (CA INDEX NAME)

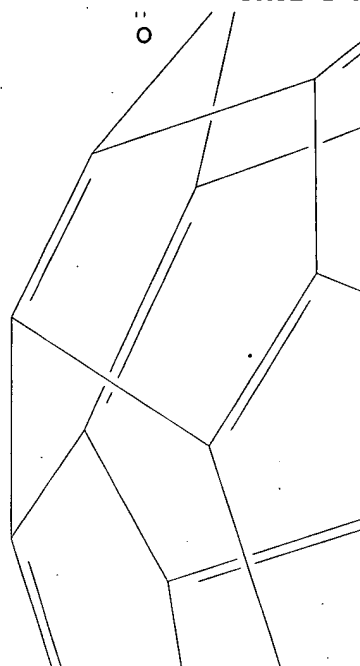
PAGE 1-A



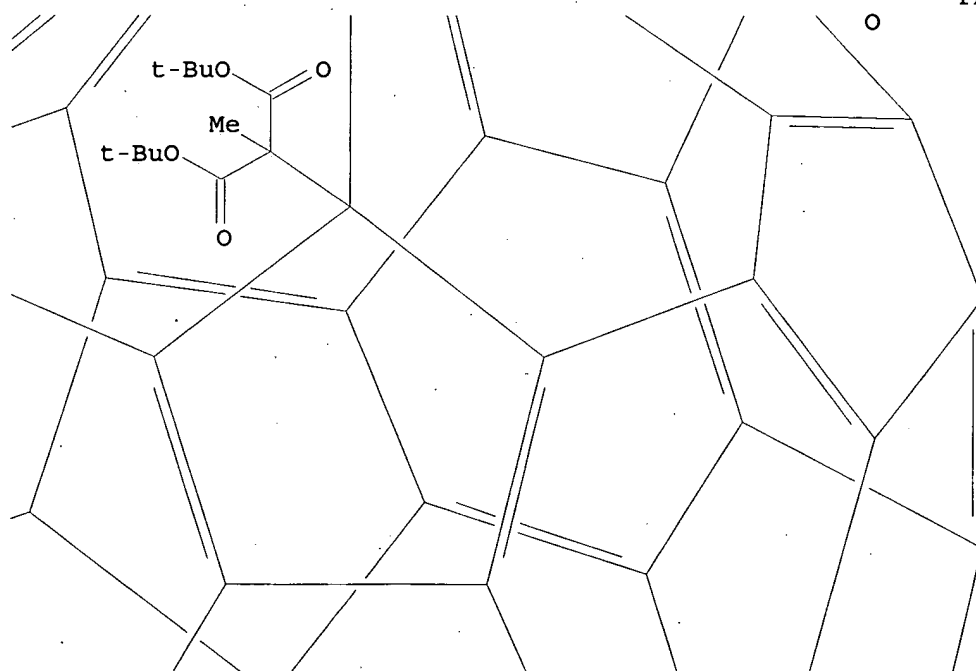
PAGE 1-B



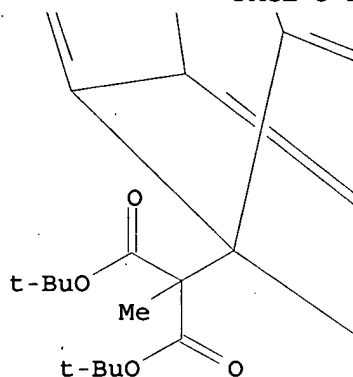
PAGE 2-A



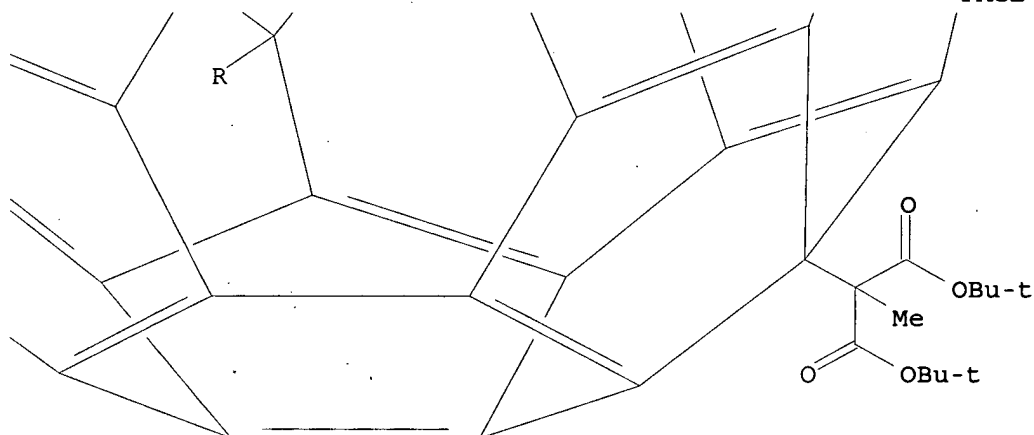
PAGE 2-B



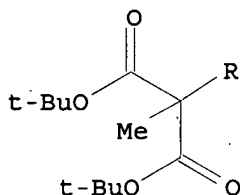
PAGE 3-A



PAGE 3-B



PAGE 4-A



CC 73-4 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)  
Section cross-reference(s): 25  
IT 836649-07-1P 836649-08-2P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(intense near-IR optical absorbing emerald green [60]Fullerenes)  
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 9 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:1013677 HCAPLUS

DOCUMENT NUMBER: 142:134293

TITLE: Manganese(III) acetate-mediated free radical reactions of [60]fullerene with  $\beta$ -dicarbonyl compounds

AUTHOR(S): Li, Changzhi; Zhang, Danwei; Zhang, Xiaotong; Wu, Shihui; Gao, Xiang

CORPORATE SOURCE: Department of Chemistry, Fudan University, Shanghai, 200433, Peop. Rep. China

SOURCE: Organic &amp; Biomolecular Chemistry (2004), 2(23), 3464-3469

CODEN: OBCRAK; ISSN: 1477-0520

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:134293

AB [60]Fullerene reacted with various  $\beta$ -dicarbonyl compds. in the presence of  $\text{Mn}(\text{OAc})_3 \cdot 2\text{H}_2\text{O}$  to generate dihydrofuran-fused [60]fullerene derivs. or 1,4-bisadducts. Dihydrofuran-fused [60]fullerene derivs. could be formed by treatment of  $\alpha$ -unsubstituted  $\beta$ -diketones or  $\beta$ -ketoesters with [60]fullerene in refluxing chlorobenzene in the presence of  $\text{Mn}(\text{III})$ . Solvent-participated unsym. 1,4-bisadducts were obtained through the reaction of [60]fullerene with di-Me malonate or  $\alpha$ -substituted  $\beta$ -dicarbonyl compds. in toluene. A possible reaction mechanism for the formation of different fullerene derivs. is proposed.

IT 666837-12-3P

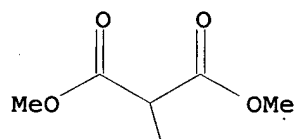
RL: SPN (Synthetic preparation); PREP (Preparation)  
(manganese(III) acetate-mediated free radical reactions of [60]fullerene with  $\beta$ -dicarbonyl compds.)

RN 666837-12-3 HCAPLUS

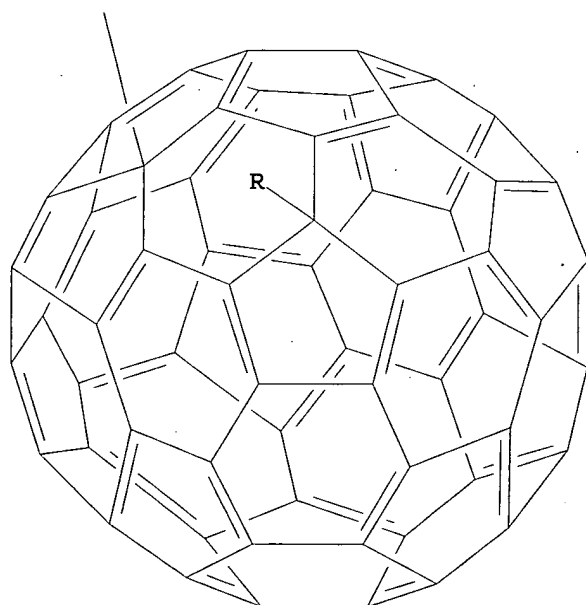
CN [5,6]Fullerene-C60-1h-1,7-diacetic acid,  $\alpha, \alpha'$ -bis(methoxycarbonyl)-, dimethyl ester (9CI) (CA INDEX NAME)



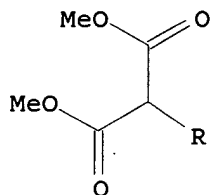
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CC 25-29 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 IT 175696-22-7P 175696-23-8P 182819-43-8P **666837-12-3P**  
 708271-04-9P 827343-33-9P 827343-41-9P 827343-44-2P  
 827343-47-5P 827343-53-3P 827343-56-6P 827343-61-3P  
 827343-67-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (manganese(III) acetate-mediated free radical reactions of  
 [60]fullerene with  $\beta$ -dicarbonyl compds.)

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE  
 FOR THIS RECORD. ALL CITATIONS AVAILABLE  
 IN THE RE FORMAT

L12 ANSWER 10 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:539720 HCAPLUS

DOCUMENT NUMBER: 141:243279

TITLE: Synthesis of [60]Fullerene Adducts Bearing  
 Carbazole Moieties by Bingel Reaction and Their  
 Properties

AUTHOR(S): Nakamura, Yosuke; Suzuki, Masato; Imai, Yumi;  
 Nishimura, Jun

CORPORATE SOURCE: Department of Nano-Material Systems, Graduate  
 School of Engineering, Gunma University, Kiryu,  
 Gunma, 376-8515, Japan

SOURCE: Organic Letters (2004), 6(16), 2797-2799

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:243279

AB Carbazole-linked [60]fullerene adducts were successfully prepared by  
 the Bingel reactions using carbazole derivs. bearing one or two Et  
 malonate moieties. In the latter cases, specific bisadduct  
 regioisomers were obtained, depending on the spacer unit between two  
 Et malonate moieties.

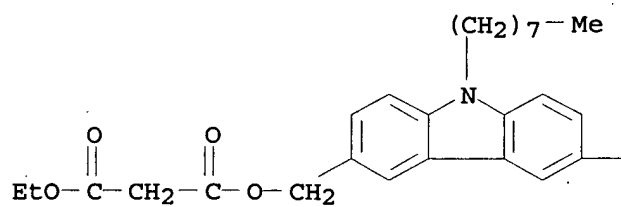
IT **748770-14-1P 748770-15-2P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of [60]fullerene adducts bearing carbazole moieties by  
 Bingel reaction and their properties)

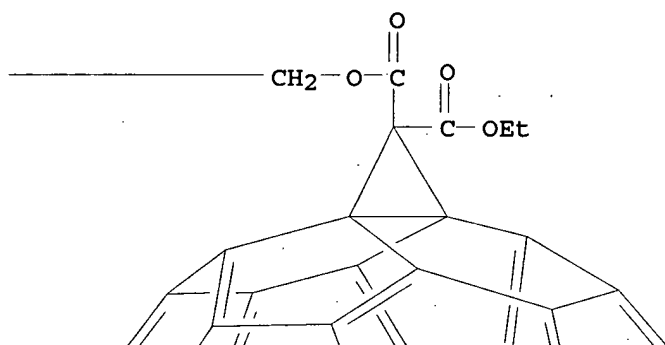
RN 748770-14-1 HCAPLUS

CN 3'H-Cyclopropa[1,9][5,6]fullerene-C60-1h-3',3'-dicarboxylic acid,  
 [6-[(3-ethoxy-1,3-dioxopropoxy)methyl]-9-octyl-9H-carbazol-3-  
 yl)methyl ethyl ester (9CI) (CA INDEX NAME)

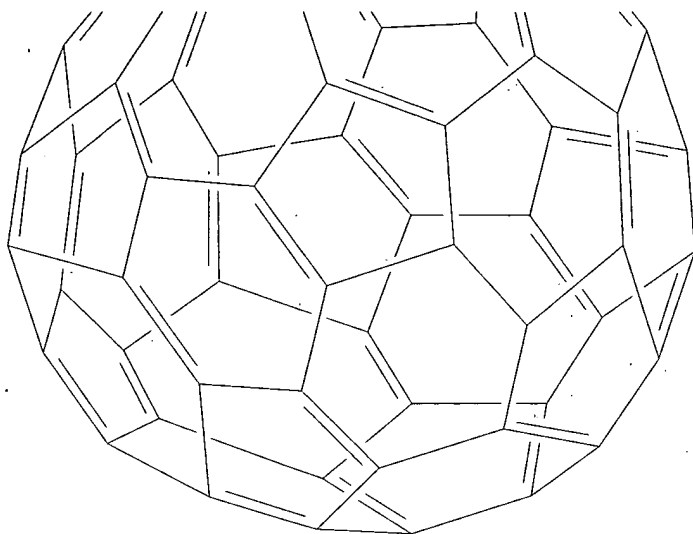
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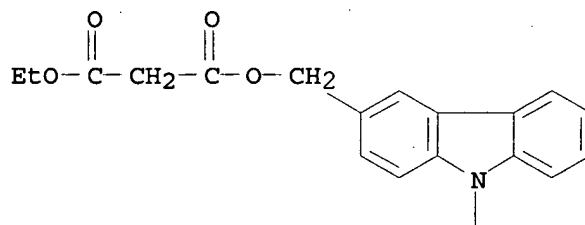


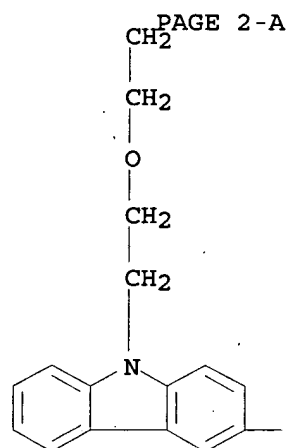
PAGE 2-B



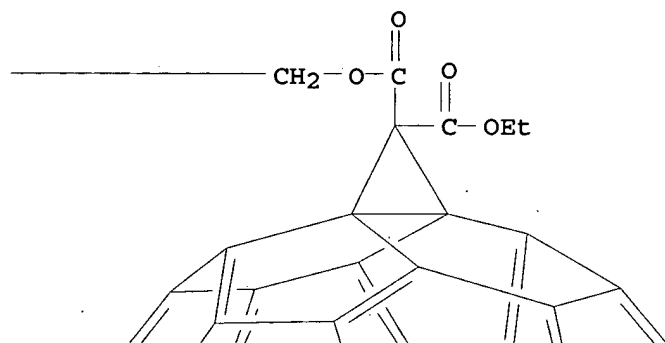
RN 748770-15-2 HCAPLUS  
CN 3'H-Cyclopropa[1,9][5,6]fullerene-C60-1h-3',3'-dicarboxylic acid,  
[9-[2-[2-[3-[(3-ethoxy-1,3-dioxopropoxy)methyl]-9H-carbazol-9-yl]ethoxy]ethyl]-9H-carbazol-3-yl]methyl ethyl ester (9CI) (CA  
INDEX NAME)

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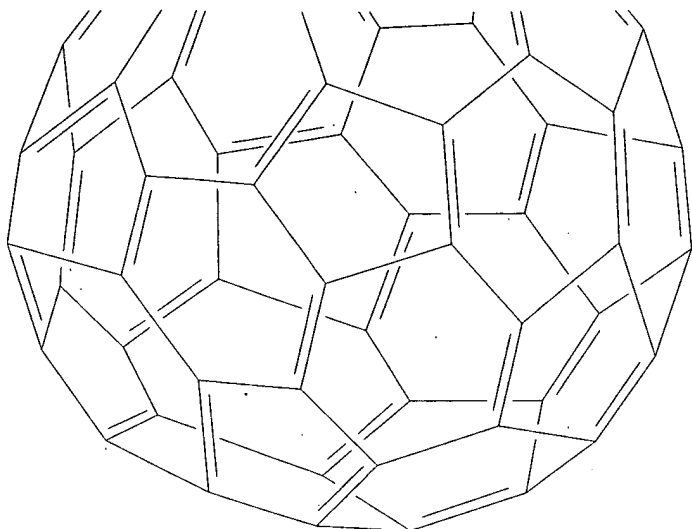




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CC 27-11 (Heterocyclic Compounds (One Hetero Atom))  
Section cross-reference(s): 25  
IT 748770-14-1P 748770-15-2P 749240-24-2P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of [60]fullerene adducts bearing carbazole moieties by  
Bingel reaction and their properties)  
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE  
FOR THIS RECORD. ALL CITATIONS AVAILABLE  
IN THE RE FORMAT

L12 ANSWER 11 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2004:462229 HCAPLUS  
DOCUMENT NUMBER: 141:190586  
TITLE: Solvent-free reactions of C60 with active  
methylene compounds, either with or without  
carbon tetrabromide, in the presence of bases  
under high-speed vibration milling conditions  
AUTHOR(S): Zhang, Ting-Hu; Wang, Guan-Wu; Lu, Ping; Li,  
Yu-Jin; Peng, Ru-Fang; Liu, You-Cheng; Murata,  
Yasujiro; Komatsu, Koichi  
CORPORATE SOURCE: Department of Chemistry, University of Science  
and Technology of China, Hefei, Peop. Rep. China  
SOURCE: Organic & Biomolecular Chemistry (2004), 2(12),  
1698-1702  
CODEN: OBCRAK; ISSN: 1477-0520  
PUBLISHER: Royal Society of Chemistry  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 141:190586  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Solvent-free reactions of C60 with active methylene compds., either

with or without carbon tetrabromide (CBr<sub>4</sub>), in the presence of a base under high-speed vibration milling (HSVM) conditions were investigated. The reaction of C<sub>60</sub> with di-Et bromomalonate was conducted under HSVM conditions in the presence of piperidine, triethylamine or Na<sub>2</sub>CO<sub>3</sub> to afford cyclopropane derivative I (R<sub>1</sub> = R<sub>2</sub> = CO<sub>2</sub>Et). In the presence of CBr<sub>4</sub>, methanofullerenes I (R<sub>1</sub> = R<sub>2</sub> = CO<sub>2</sub>Et or CO<sub>2</sub>Me; R<sub>1</sub> = COMe or CN, R<sub>2</sub> = CO<sub>2</sub>Et) could be obtained by the direct reaction of C<sub>60</sub> with di-Et malonate, di-Me malonate, Et acetoacetate and Et cyanoacetate, resp., with the aid of 1,8-diazabicyclo[5,4,0]undec-7-ene, piperidine, triethylamine or Na<sub>2</sub>CO<sub>3</sub>. More interestingly, 1,4-bisadducts II (R = Et, Me) were produced by the reaction of C<sub>60</sub> with di-Et malonate and di-Me malonate in the presence of piperidine, triethylamine or Na<sub>2</sub>CO<sub>3</sub> under HSVM conditions. On the other hand, dihydrofuran-fused C<sub>60</sub> derivs. III (R<sub>1</sub> = Me, R<sub>2</sub> = OEt or Me; R<sub>1</sub> = R<sub>2</sub> = CH<sub>2</sub>CMe<sub>2</sub>CH<sub>2</sub>) were obtained from the reaction of C<sub>60</sub> with Et acetoacetate, 2,4-pentanedione and 5,5-dimethyl-1,3-cyclohexanedione with the aid of a base. Under the same conditions, less activated aryl Me ketones such as 2-acetylpyridine, 2-acetylpyrazine and acetophenone provided monocarbonylated methanofullerene derivs. IV (X = N, Y = C; X = Y = N or C). Except for the Bingel reactions, all other reactions under the HSVM conditions are considered to proceed according to a single-electron-transfer mechanism.

IT 573951-18-5P 666837-12-3P

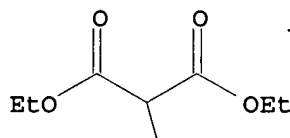
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of substituted fullerenes via solvent-free reactions of C<sub>60</sub> with active methylene compds., either with or without carbon tetrabromide, in the presence of bases under high-speed vibration milling conditions)

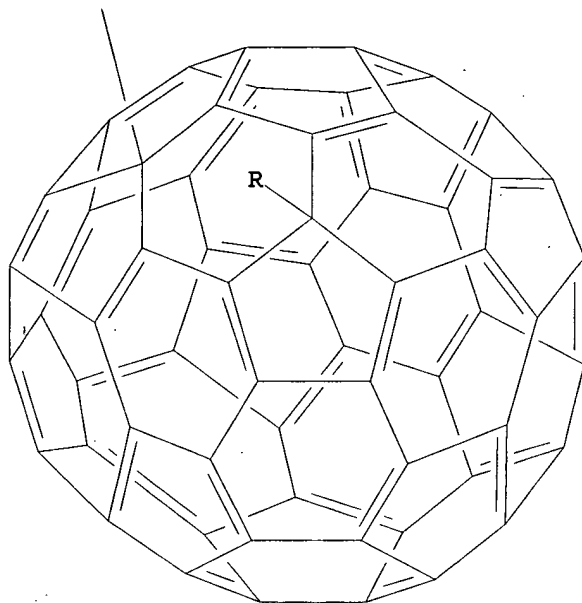
RN 573951-18-5 HCAPLUS

CN [5,6]Fullerene-C<sub>60</sub>-1h-1,7-diacetic acid,  $\alpha,\alpha'$ -bis(ethoxycarbonyl)-, diethyl ester (9CI) (CA INDEX NAME)

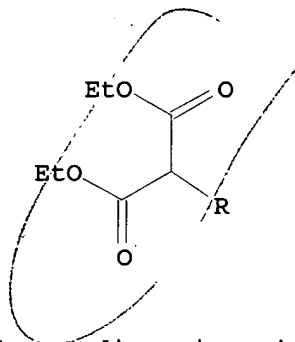
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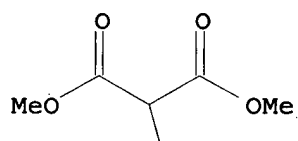
PAGE 3-A



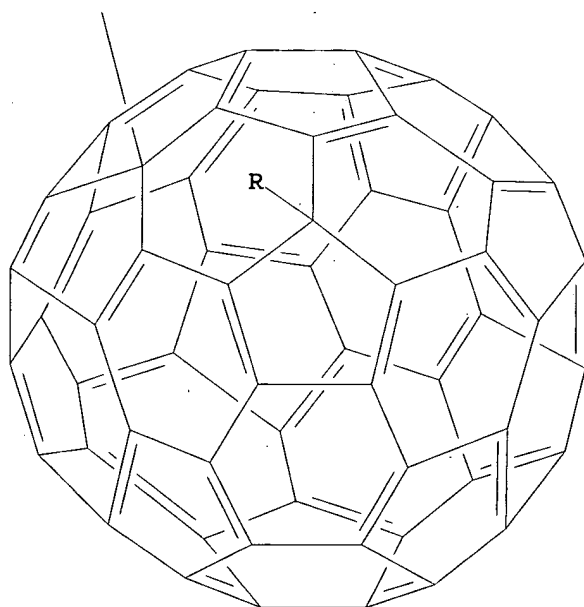
RN 666837-12-3 HCAPLUS  
CN [5,6]Fullerene-C60-1h-1,7-diacetic acid,  $\alpha,\alpha'$ -  
bis(methoxycarbonyl)-, dimethyl ester (9CI) (CA INDEX NAME)



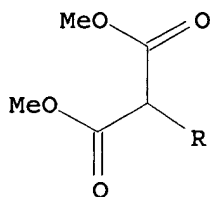
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CC 25-29 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
IT 153218-90-7P 153218-92-9P 175696-19-2P 175696-22-7P  
176961-89-0P 182819-43-8P 188409-02-1P 207684-19-3P  
573951-18-5P 666837-12-3P 710316-31-7P  
736980-91-9P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of substituted fullerenes via solvent-free reactions of  
C60 with active methylene compds., either with or without carbon  
tetrabromide, in the presence of bases under high-speed vibration  
milling conditions)

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE  
FOR THIS RECORD. ALL CITATIONS AVAILABLE  
IN THE RE FORMAT

L12 ANSWER 12 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:75249 HCAPLUS

DOCUMENT NUMBER: 140:356916

TITLE: Design and synthesis of multi-component 18 $\pi$   
annulenic fluorofullerene ensembles suitable for  
donor-acceptor applications

AUTHOR(S): Burley, Glenn A.; Avent, Anthony G.; Gol'dt,  
Ilya V.; Hitchcock, Peter B.; Al-Matar, Hamad;  
Paolucci, Demis; Paolucci, Francesco; Fowler,  
Patrick W.; Soncini, Alessandro; Street, Joan  
M.; Taylor, Roger

CORPORATE SOURCE: Chemistry Department, University of Sussex,  
Brighton, BN1 9QJ, UK

SOURCE: Organic & Biomolecular Chemistry (2004), 2(3),  
319-329

CODEN: OBCRAK; ISSN: 1477-0520

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:356916

AB A series of trannulene (all-trans annulene) derivs. of [60]fullerene  
have been prepared by reacting C60F18 with methanetricarboxylate  
esters that incorporate a range of photoactive functions. All the  
compds. have the intense emerald-green color of fullerene  
trannulenes, characterized by strong bands at ca. 612 and 667 nm.  
Single crystal X-ray studies show that the packing varies with the  
nature of the addend, attributable to differing steric effects.  
UV/vis absorption spectra display transitions of the resp. fullerene  
and addend models, indicating absence of electronic interactions  
between them in the ground state. These now provide an extensive  
series for testing photoactive (light-harvesting) properties, with  
the exceptional properties of having strong visible light  
absorption. Their exceptional stability is attributed to the 18 $\pi$   
aromatic circuit, inability to undergo nucleophilic substitution  
without disrupting this circuit, and a curved cage region that is

shielded to reagents by the three bulky addends.

IT 681846-24-2  
RL: PRP (Properties)  
(crystal structure; design and synthesis of multi-component  
18 $\pi$ -annulenic fluorofullerene ensembles suitable for  
donor-acceptor applications)

RN 681846-24-2 HCAPLUS  
CN [5,6]Fullerene-C60-Ih-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha,\alpha',\alpha',\alpha'',\alpha''$ -  
hexakis(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
tetradecahydro-, triethyl ester, compd. with trichloromethane-d  
(1:2) (9CI) (CA INDEX NAME)

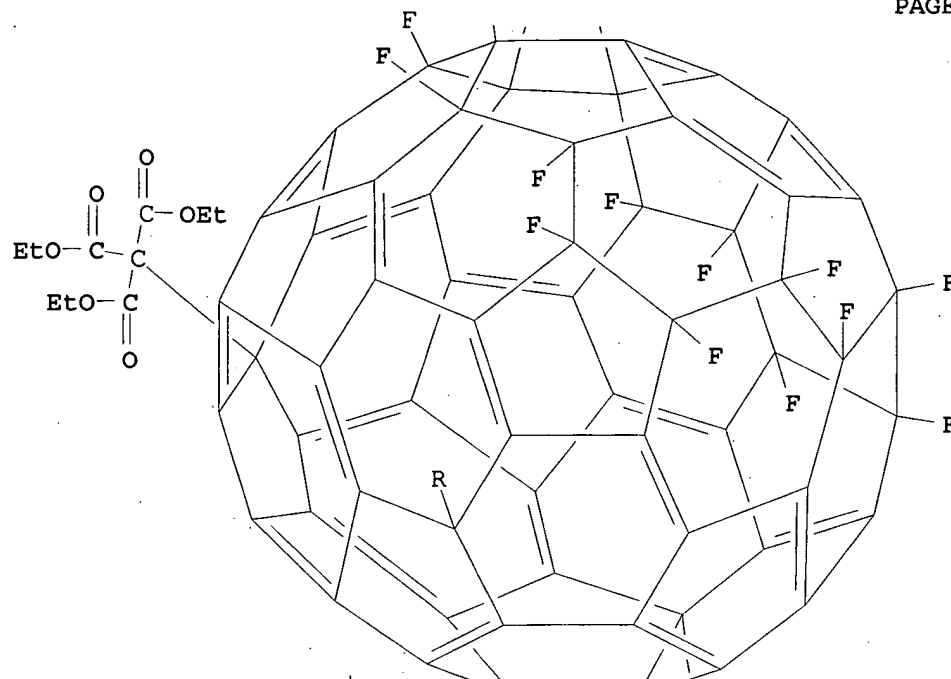
CM 1

CRN 539825-96-2  
CMF C90 H45 F15 O18

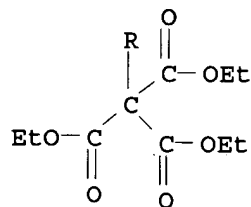
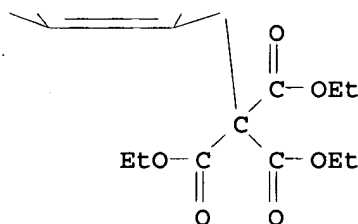
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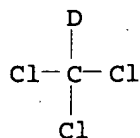
PAGE 3-A



CM 2

CRN 865-49-6

CMF C Cl3 D



IT 539825-95-1P 658065-04-4P 658065-05-5P

658065-06-6P 681846-11-7P 681846-12-8P

681846-13-9P 681846-14-0P

RL: PRP (Properties); SPN (Synthetic preparation); PREP  
(Preparation)(design and synthesis of multi-component  $18\pi$ -annulenic  
fluorofullerene ensembles suitable for donor-acceptor  
applications)

RN 539825-95-1 HCAPLUS

CN [5,6]Fullerene-C60-1h-1,33,38(23H)-triacetic acid,

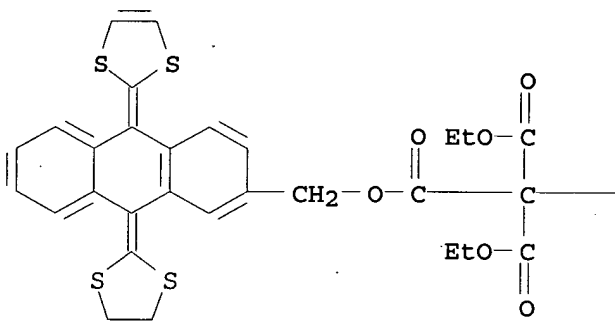
 $\alpha,\alpha,\alpha',\alpha',\alpha'',\alpha''$ -

hexakis(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-

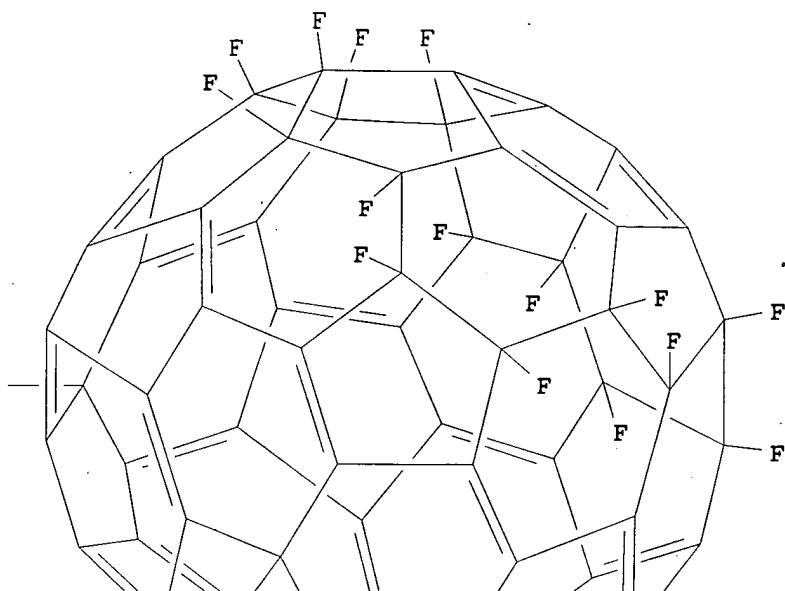
pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-

tetradecahydro-, tris[[9,10-bis(1,3-dithiol-2-ylidene)-9,10-dihydro-  
2-anthracenyl]methyl] ester (9CI) (CA INDEX NAME)

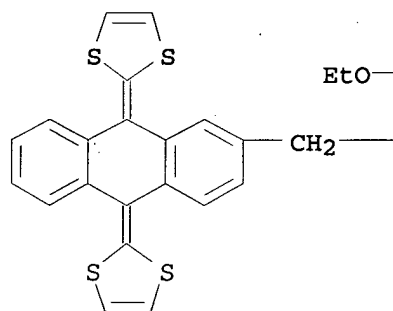
PAGE 1-A



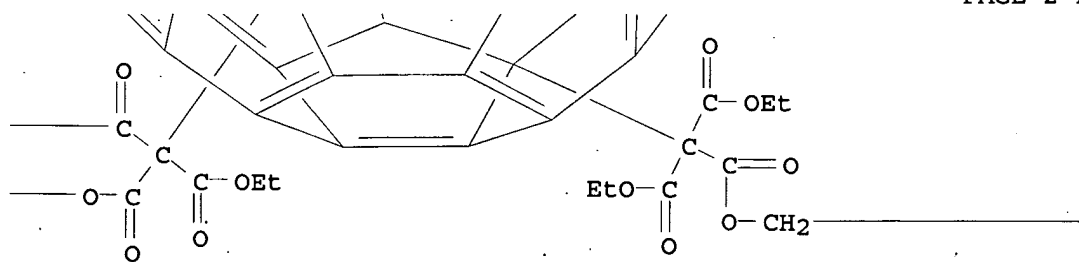
PAGE 1-B



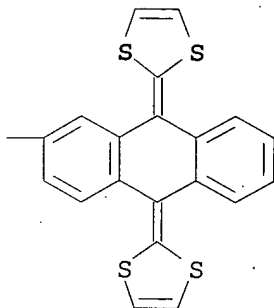
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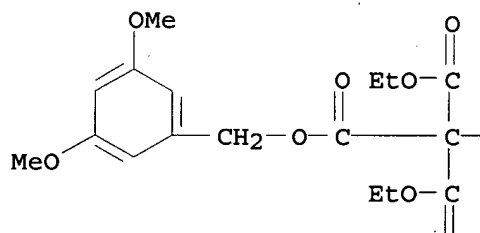


PAGE 2-C

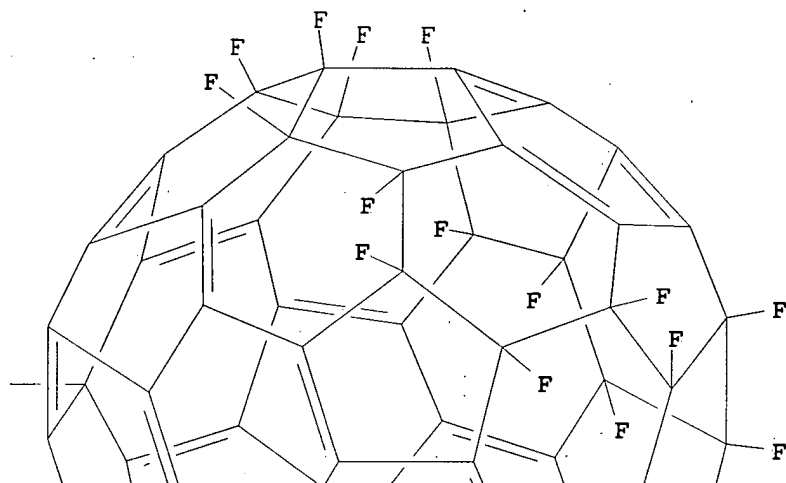


RN 658065-04-4 HCAPLUS  
 CN [5,6]Fullerene-C60-Ih-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha,\alpha',\alpha',\alpha'',\alpha''$ -  
 hexakis(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 tetradecahydro-, tris[(3,5-dimethylphenyl)methyl] ester (9CI) (CA  
 INDEX NAME)

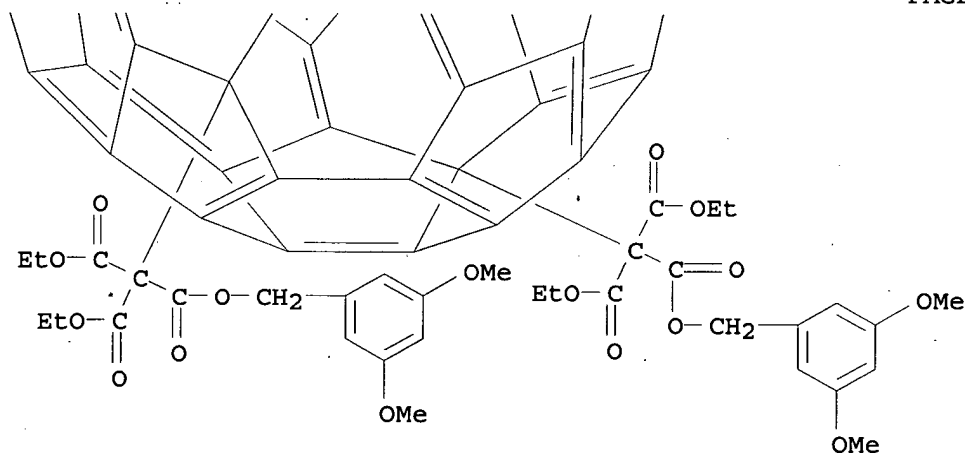
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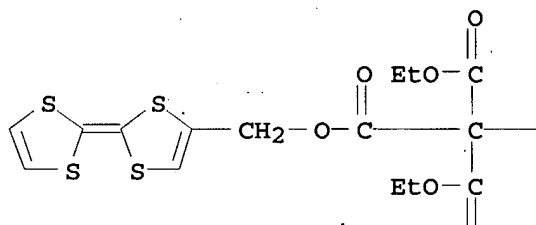


RN 658065-05-5 HCAPLUS  
 CN [5,6]Fullerene-C60-1h-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha,\alpha',\alpha',\alpha'',\alpha''$ -  
 hexakis(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-

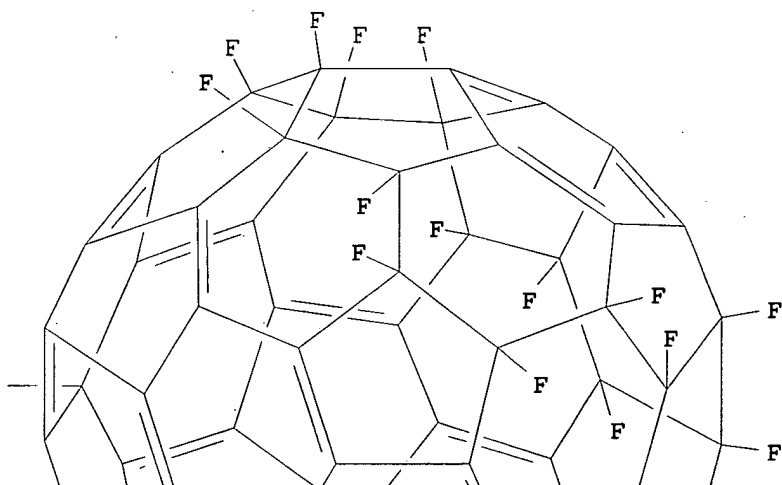


tetradecahydro-, tris[[2-(1,3-dithiol-2-ylidene)-1,3-dithiol-4-yl]methyl] ester (9CI) (CA INDEX NAME)

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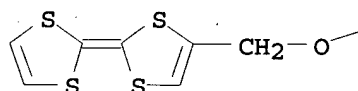
PAGE 1-B



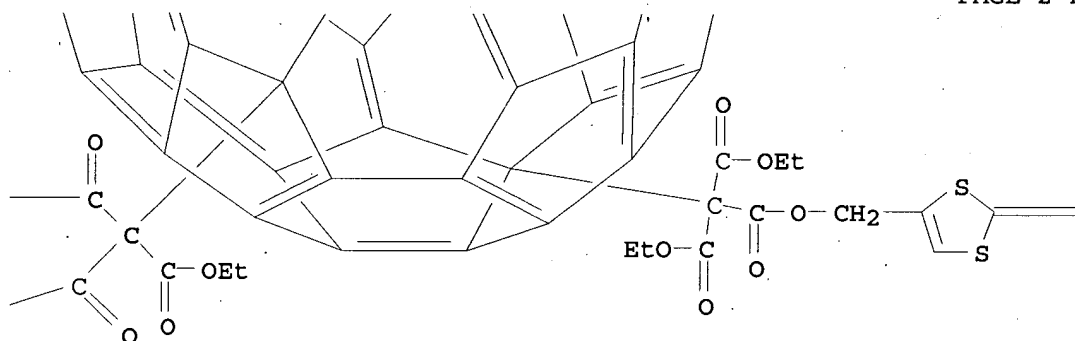
PAGE 2-A

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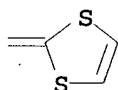
EtO—



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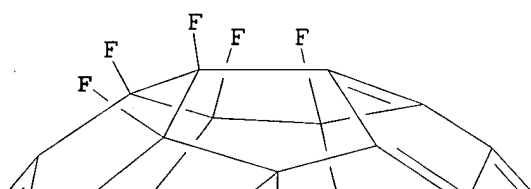


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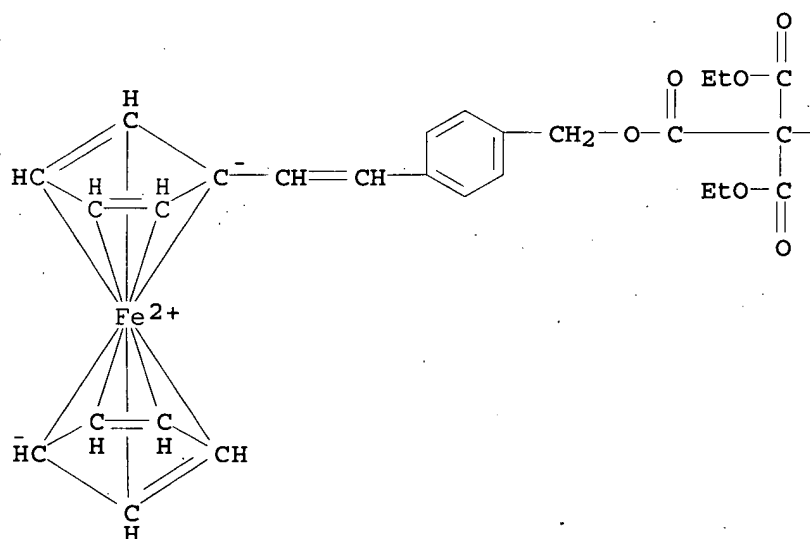


RN 658065-06-6 HCAPLUS  
 CN Ferrocene, 1,1',1''-[{(23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-tetradecahydro[5,6]fullerene-C60-Ih-1,33,38(23H)-triyl)tris[2,2-bis(ethoxycarbonyl)-1-oxo-2,1-ethanediyl]oxymethylene-4,1-phenylene-2,1-ethenediyl]]tris- (9CI) (CA INDEX NAME)

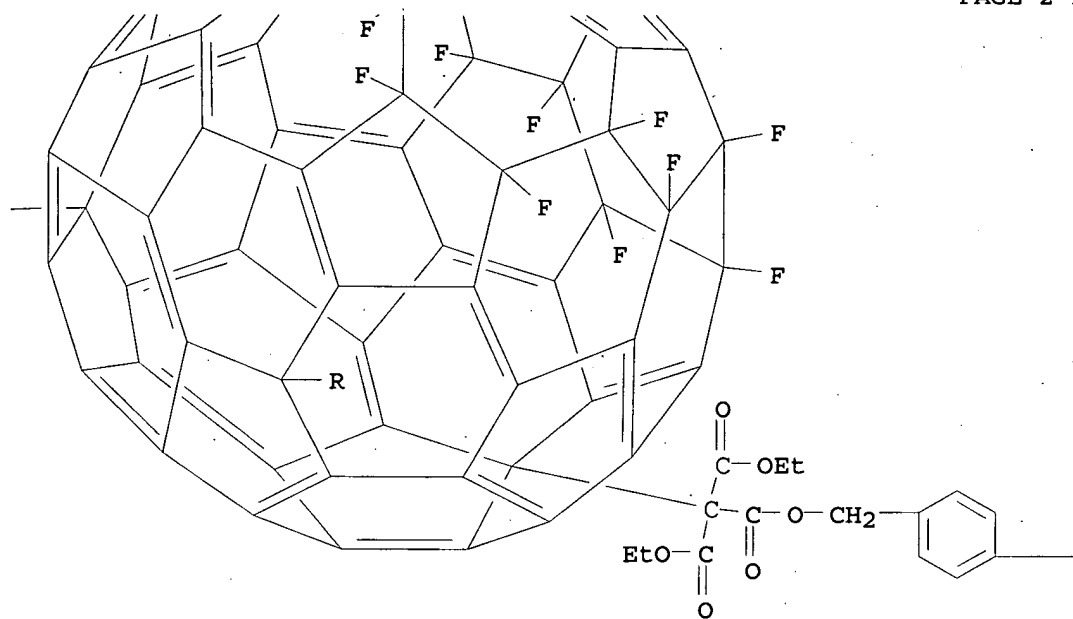
PAGE 1-B



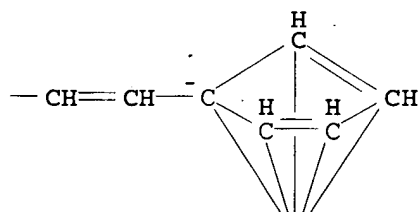
PAGE 2-A



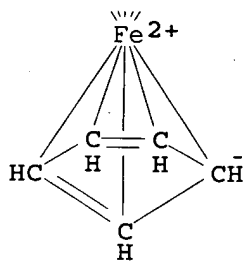
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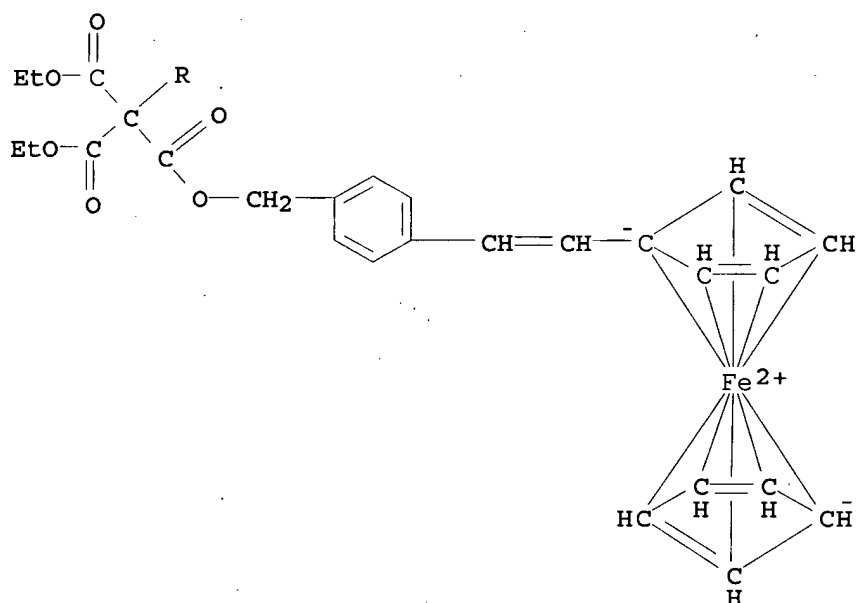
PAGE 2-C



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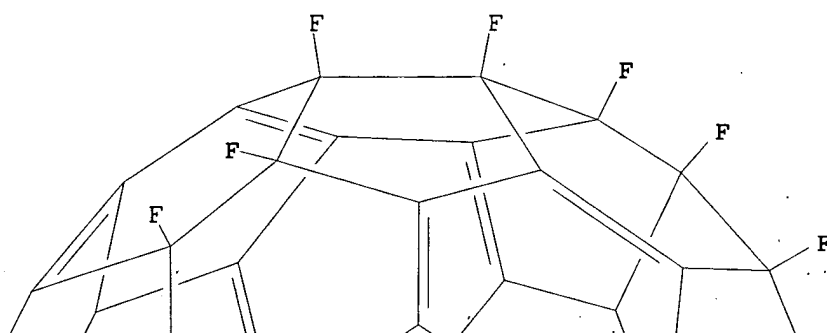


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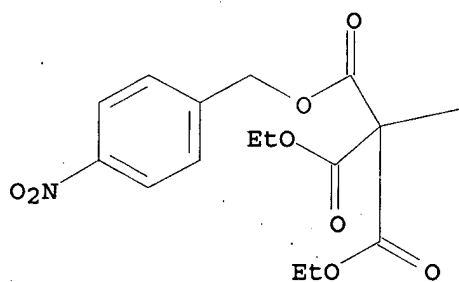


RN 681846-11-7 HCAPLUS  
 CN [5,6]Fullerene-C60-Ih-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha,\alpha',\alpha',\alpha'',\alpha''$ -  
 hexakis(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 tetradecahydro-, tris[(4-nitrophenyl)methyl] ester (9CI) (CA INDEX  
 NAME)

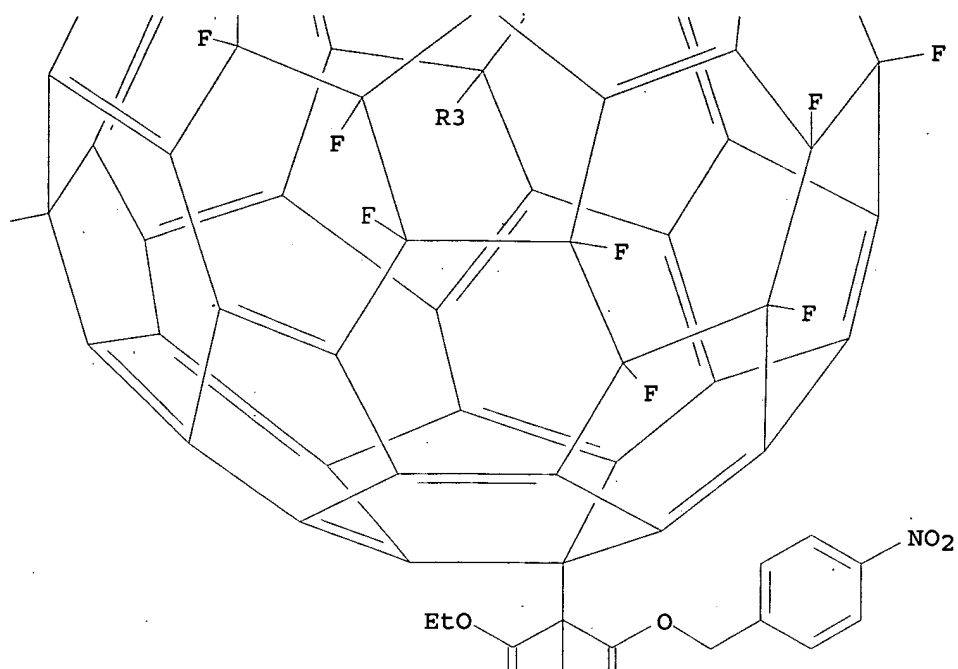
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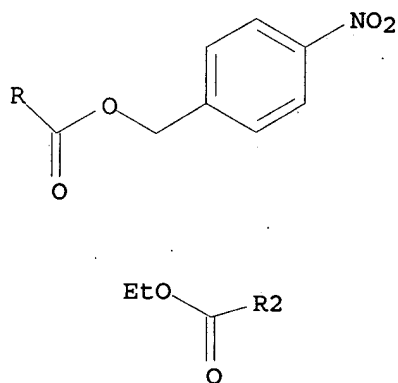
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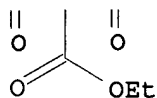
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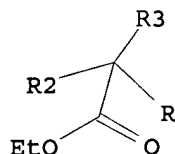
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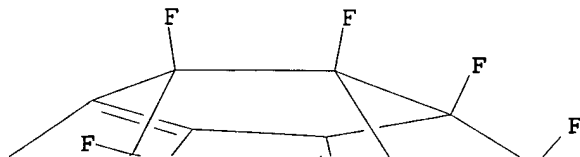


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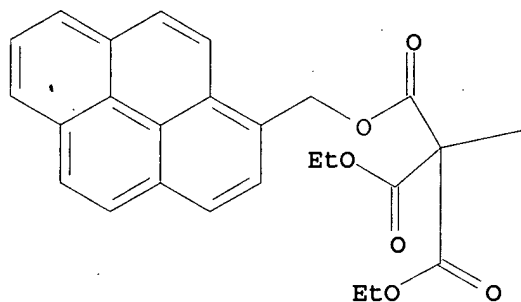
RN 681846-12-8 HCAPLUS  
 CN [5,6]Fullerene-C60-1h-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha,\alpha',\alpha',\alpha'',\alpha''$ -  
 hexakis(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 tetradecahydro-, tris(1-pyrenylmethyl) ester (9CI) (CA INDEX NAME)

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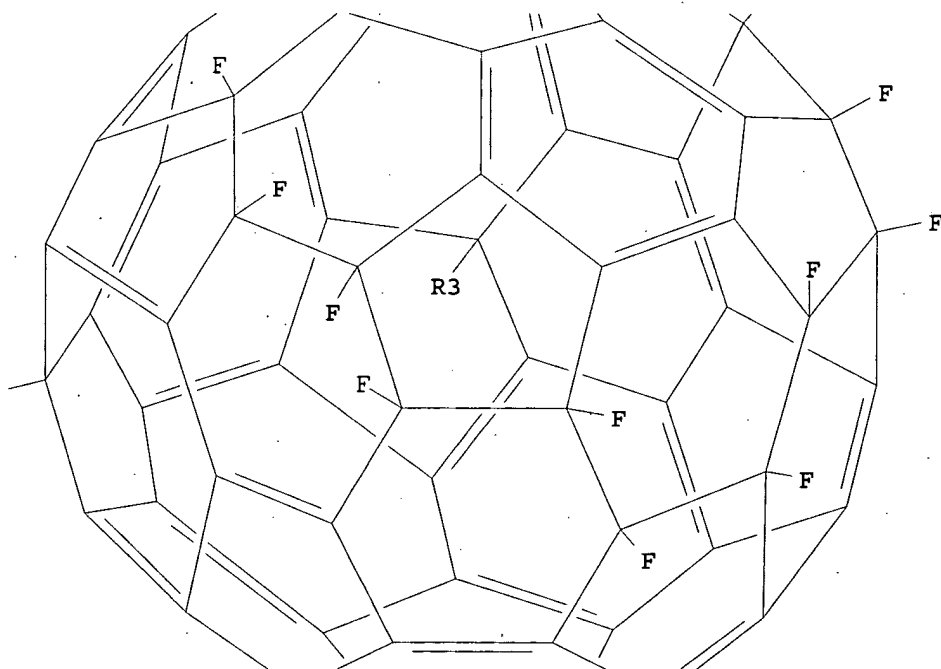




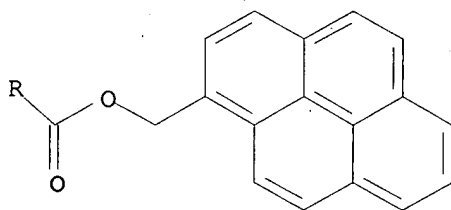
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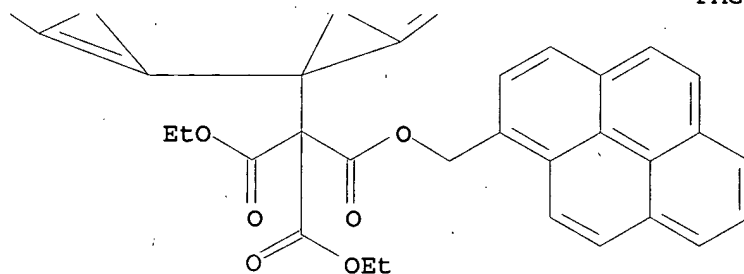
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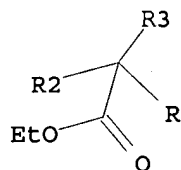
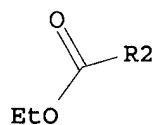
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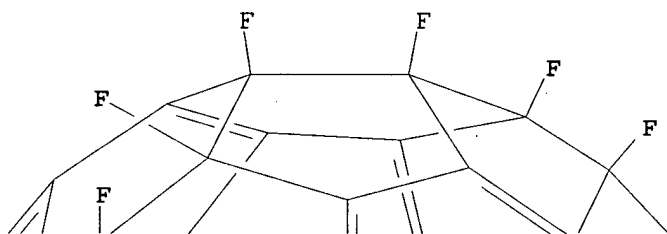
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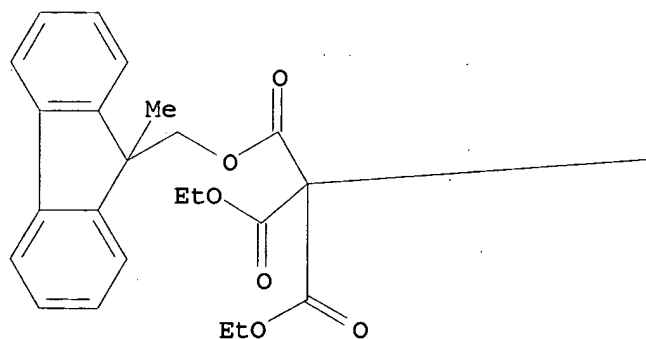
RN 681846-13-9 HCAPLUS  
CN [5,6]Fullerene-C60-Ih-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha,\alpha',\alpha',\alpha'',\alpha''$ -

hexakis(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
tetradecahydro-, tris[(9-methyl-9H-fluoren-9-yl)methyl] ester (9CI)  
(CA INDEX NAME)

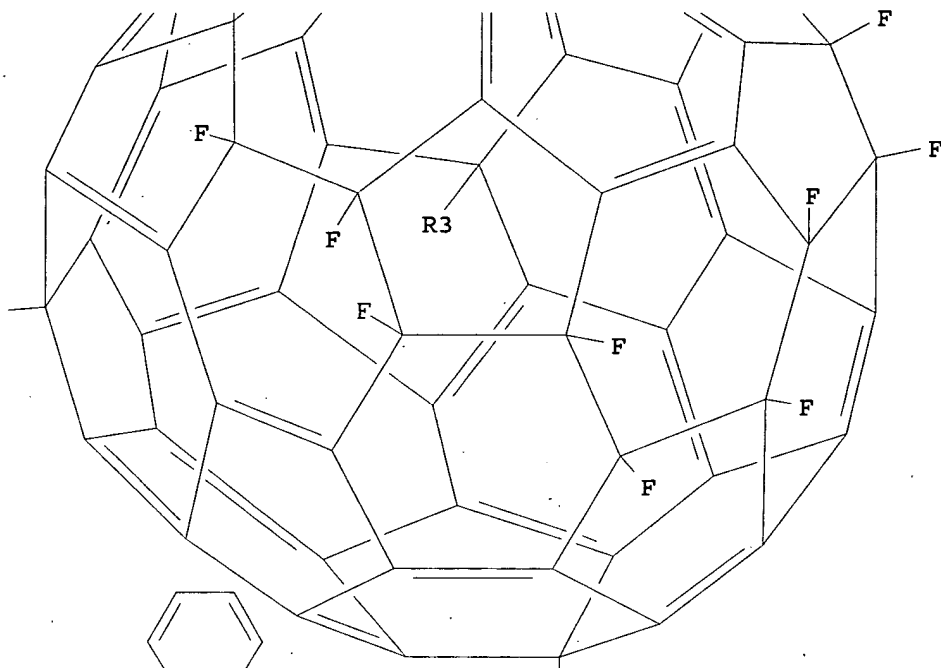
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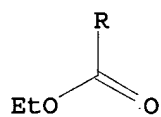


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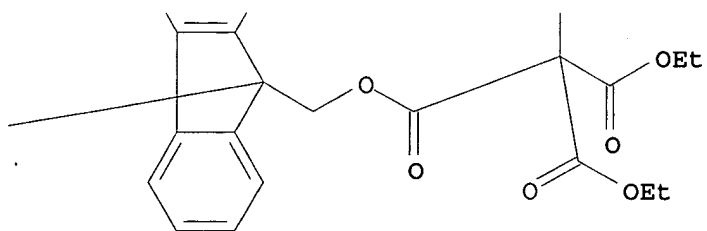


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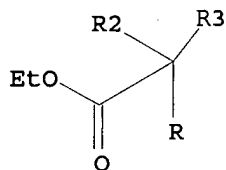
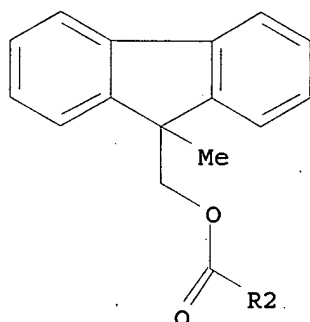
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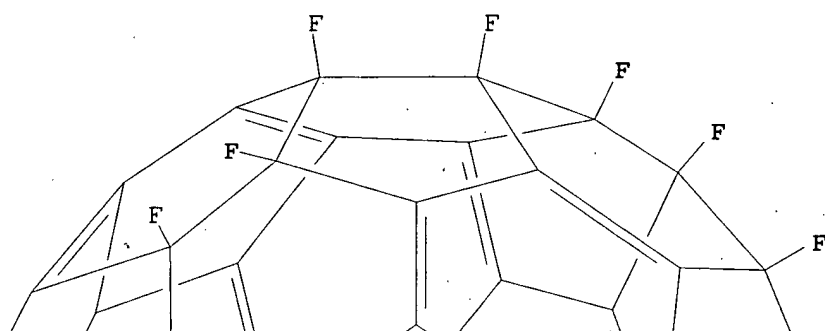


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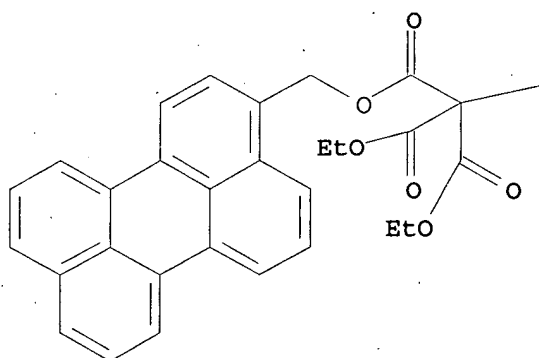


RN 681846-14-0 HCAPLUS  
CN [5,6]Fullerene-C60-Ih-1,33,38(23H)-triacetic acid,  
 $\alpha, \alpha, \alpha', \alpha', \alpha'', \alpha''$ -  
hexakis(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
tetradecahydro-, tris(3-perylenylmethyl) ester (9CI) (CA INDEX  
NAME)

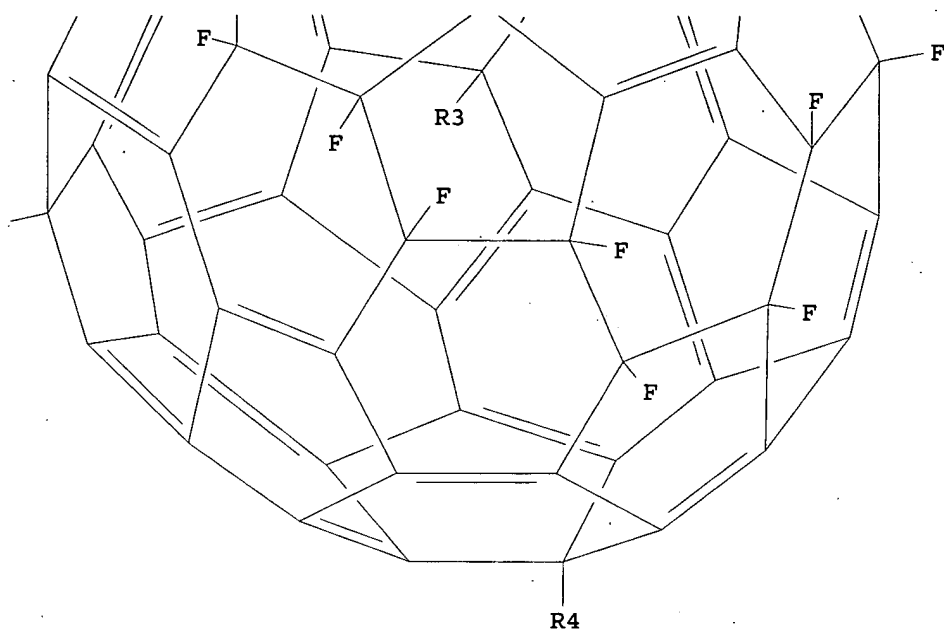
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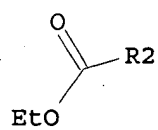
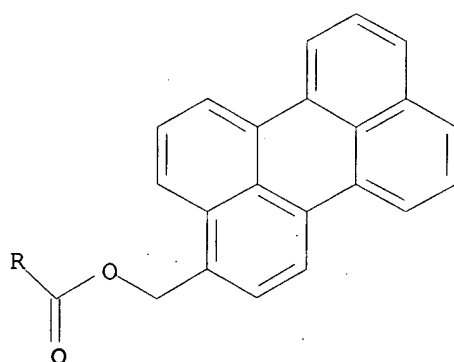
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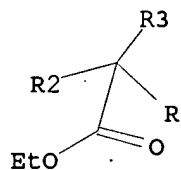
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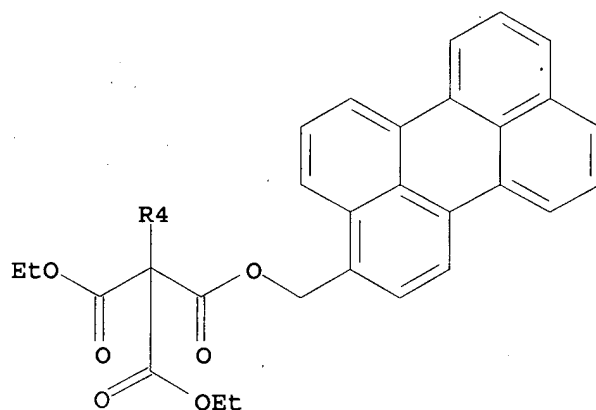
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IT 539825-96-2P 681846-21-9P 681846-23-1P

681853-89-4P 681853-90-7P

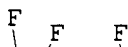
RL: SPN (Synthetic preparation); PREP (Preparation)  
 (design and synthesis of multi-component  $18\pi$ -annulenic  
 fluorofullerene ensembles suitable for donor-acceptor  
 applications)

RN 539825-96-2 HCAPLUS

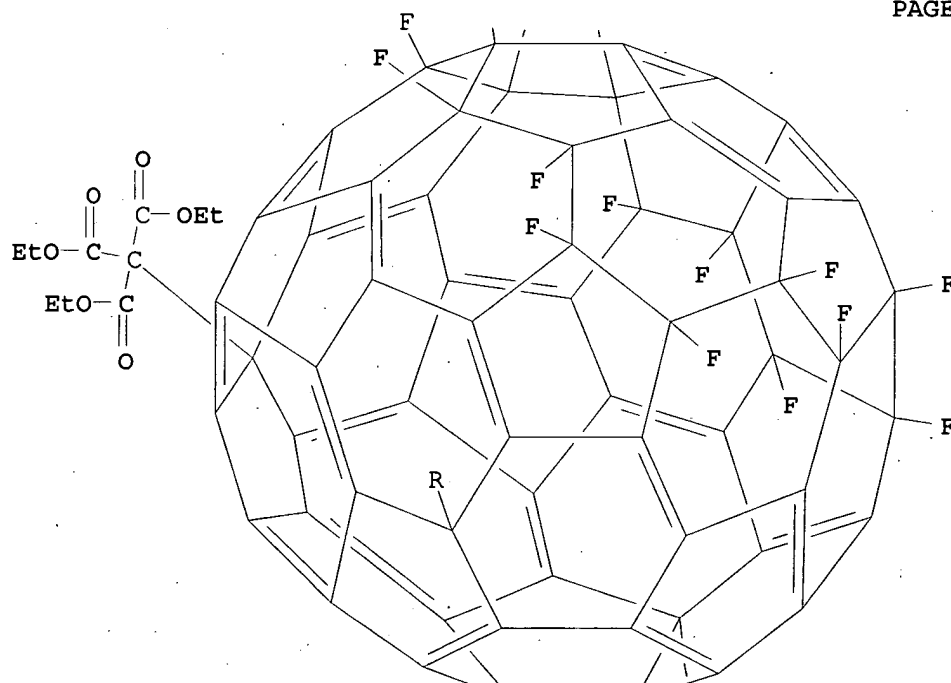
CN [5,6]Fullerene-C<sub>60</sub>-1h-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha,\alpha',\alpha',\alpha'',\alpha''$ -  
 hexakis(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 tetradecahydro-, triethyl ester (9CI) (CA INDEX NAME)



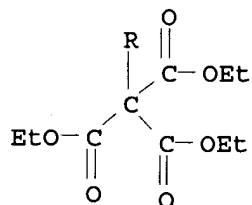
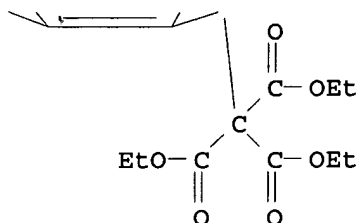
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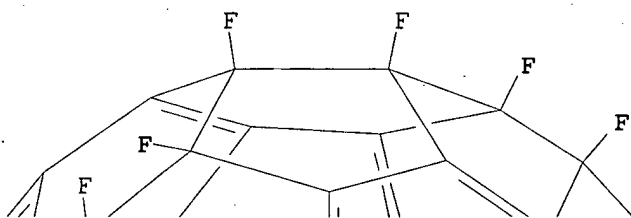


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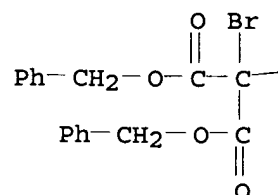


RN 681846-21-9 HCAPLUS  
 CN [5,6]Fullerene-C60-Ih-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha',\alpha''$ -tribromo-23,24,25,26,27,28,41,42,47,48,49,  
 ,55,56,59,60-pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,  
 60-tetradecahydro- $\alpha,\alpha',\alpha''$ -  
 tris[(phenylmethoxy)carbonyl]-, tris(phenylmethyl) ester (9CI) (CA  
 INDEX NAME)

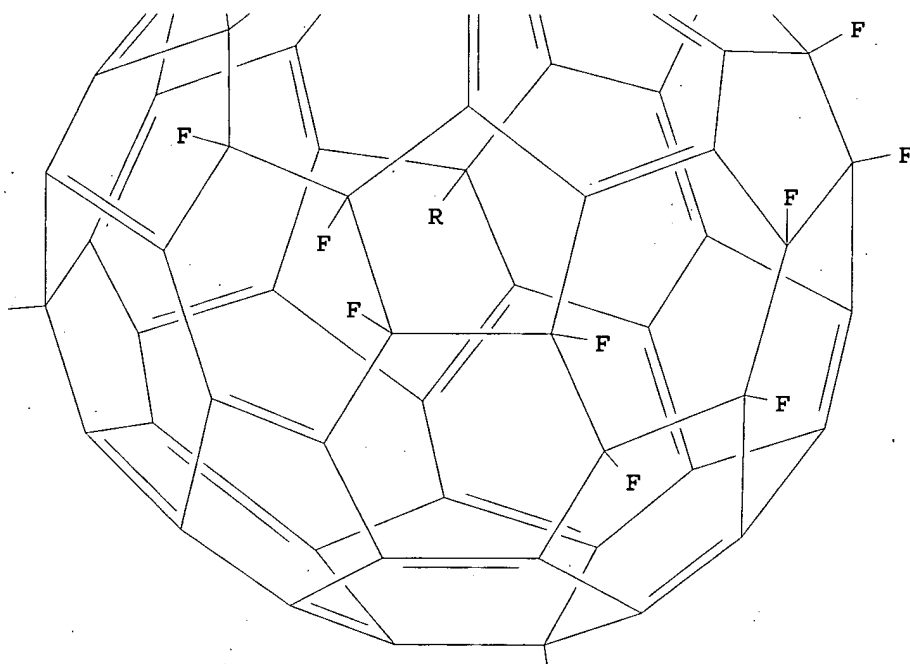
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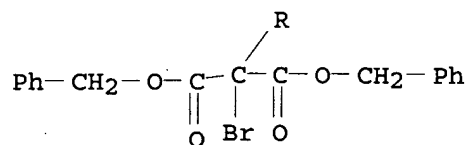
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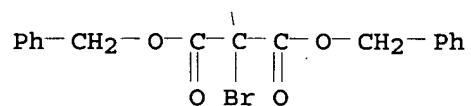
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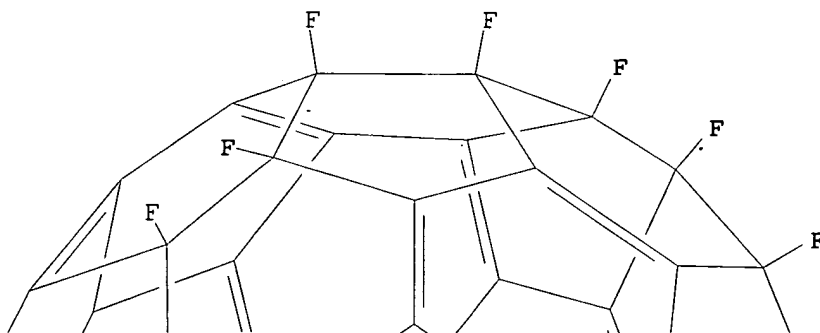


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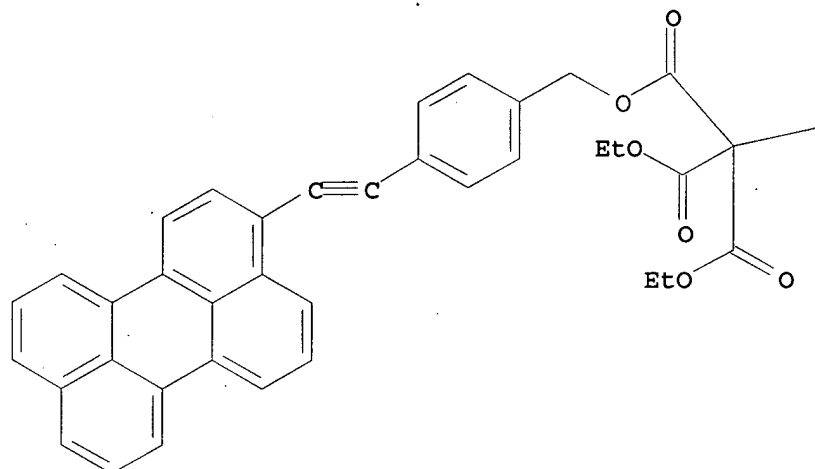


RN 681846-23-1 HCAPLUS  
 CN [5,6]Fullerene-C60-Ih-1,33,38(23H)-triacetic acid;  
 $\alpha,\alpha,\alpha',\alpha',\alpha'',\alpha''$ -  
 hexakis(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 tetradecahydro-, tris[[4-(3-perylenylethynyl)phenyl]methyl] ester  
 (9CI) (CA INDEX NAME)

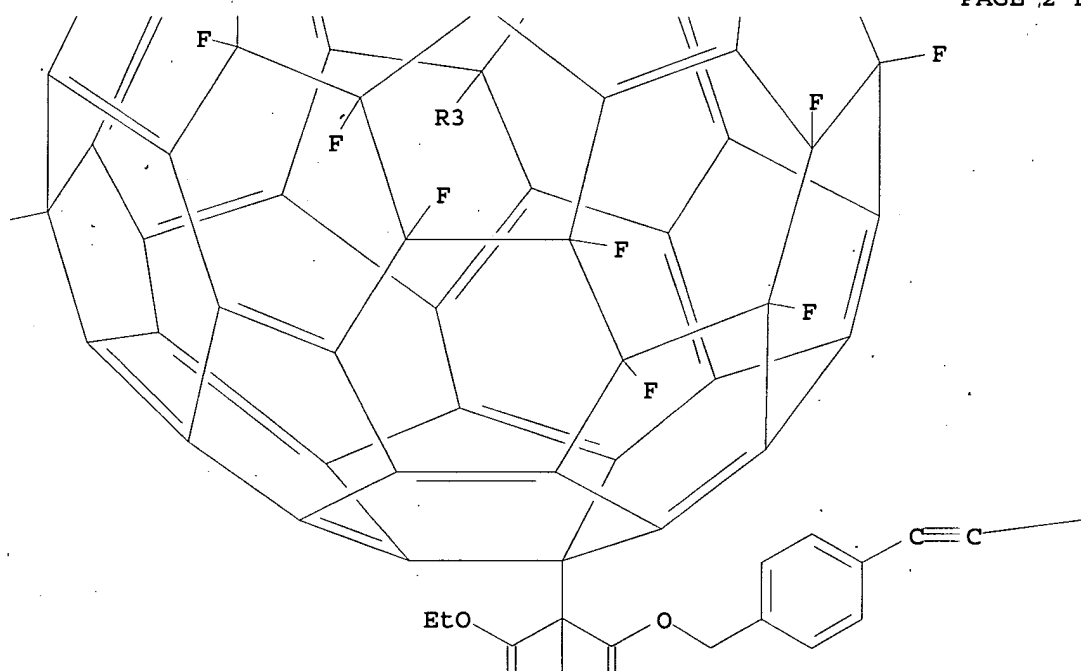
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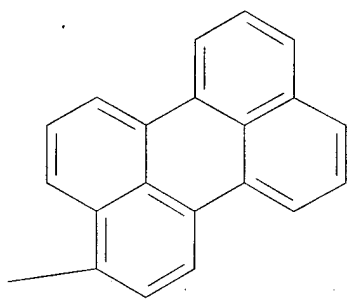
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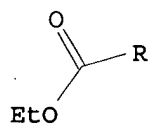
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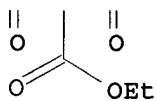
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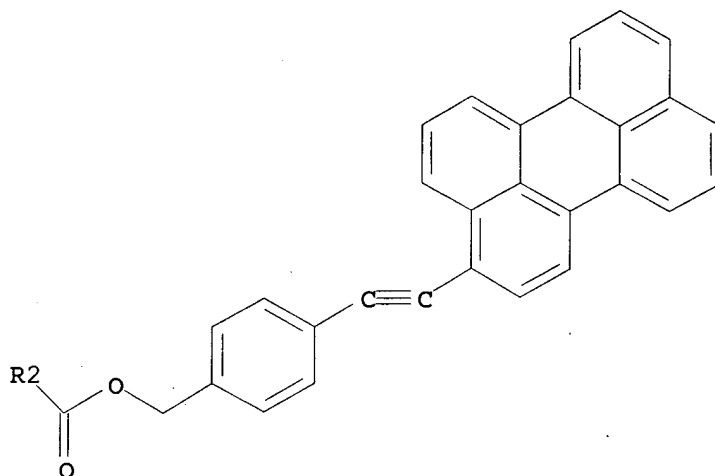
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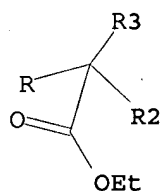
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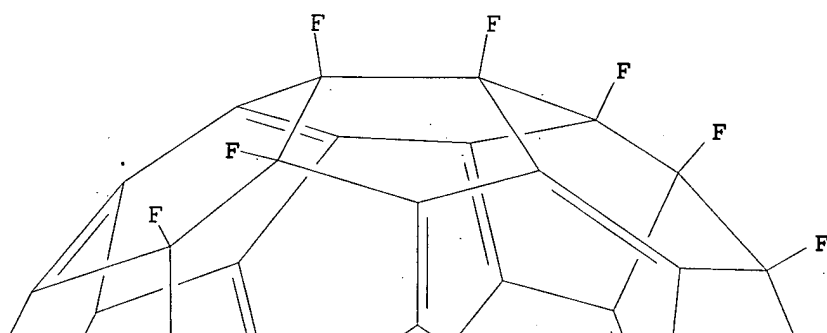


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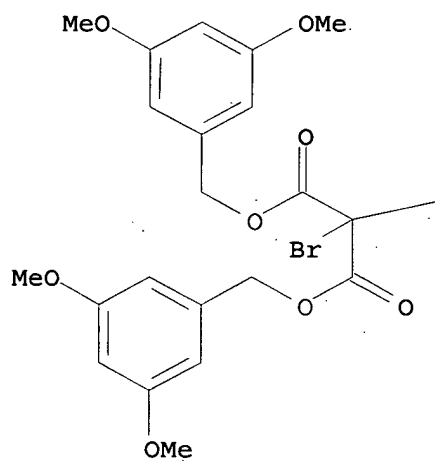


RN 681853-89-4 HCAPLUS  
CN [5,6]Fullerene-C60-1h-1,33-diacetic acid,  $\alpha,\alpha'$ -dibromo-  
 $\alpha,\alpha'$ -bis[[(3,5-dimethoxyphenyl)methoxy]carbonyl]-  
23,24,25,26,27,28,38,41,42,47,48,49,55,56,59,60-hexadecafluoro-  
23,24,25,26,27,28,38,41,42,47,48,49,55,56,59,60-hexadecahydro-,  
bis[(3,5-dimethoxyphenyl)methyl] ester (9CI) (CA INDEX NAME)

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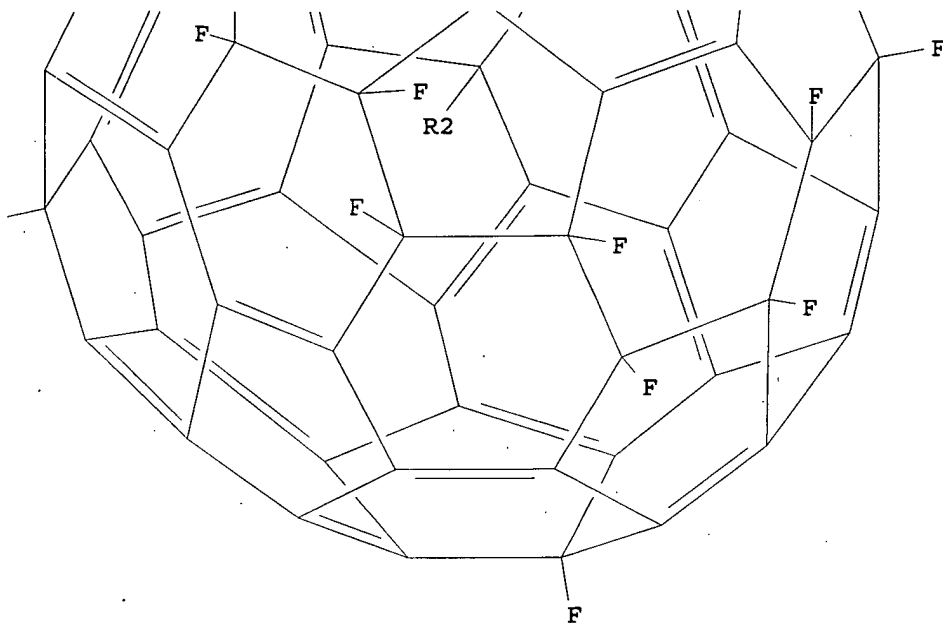


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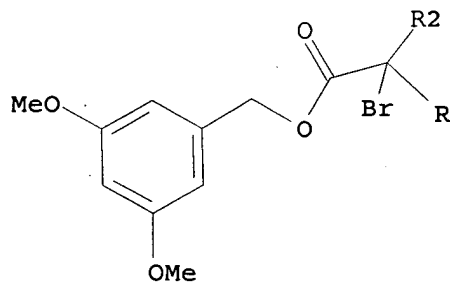
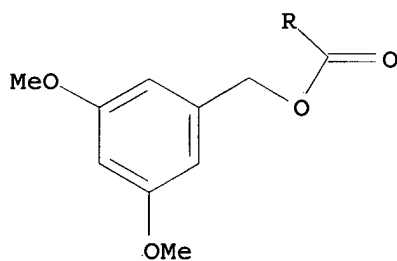




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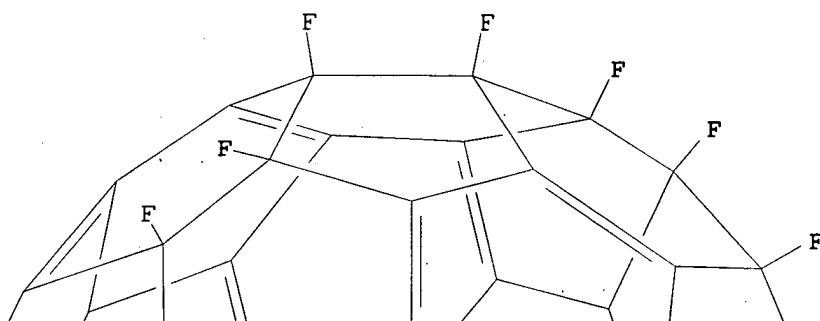


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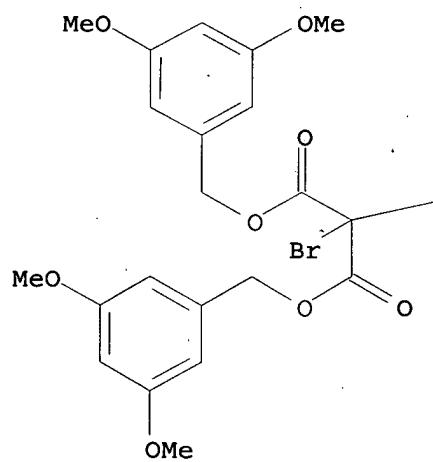


RN 681853-90-7 HCAPLUS  
 CN [5,6]Fullerene-C<sub>60</sub>-1h-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha',\alpha''$ -tribromo- $\alpha,\alpha',\alpha''$ -  
 tris[[(3,5-dimethoxyphenyl)methoxy]carbonyl]-  
 23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-pentadecafluoro-  
 24,25,26,27,28,41,42,47,48,49,55,56,59,60-tetradecahydro-,  
 tris[(3,5-dimethoxyphenyl)methyl] ester (9CI) (CA INDEX NAME)

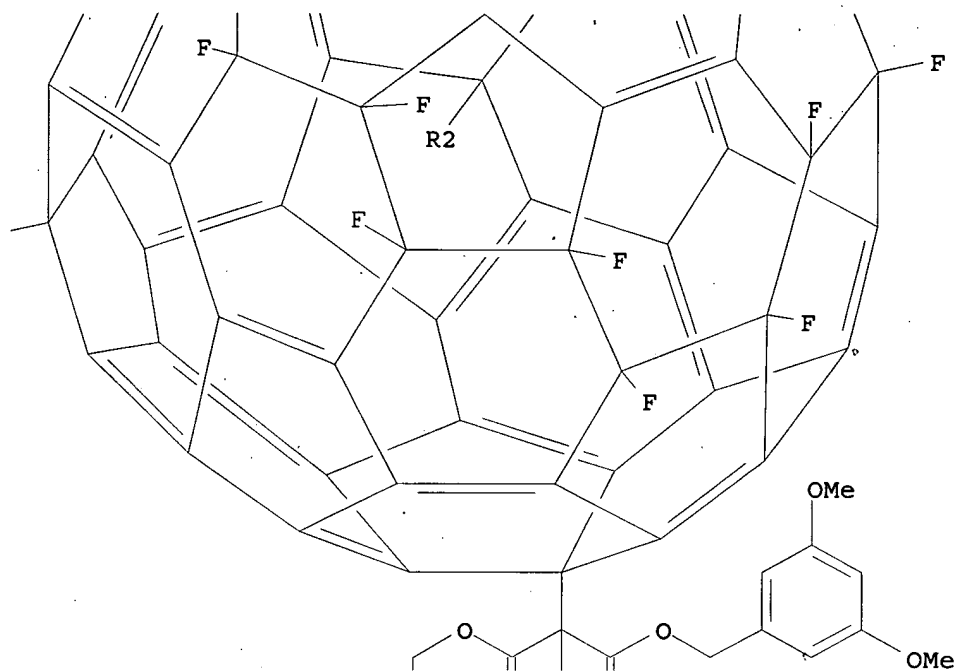
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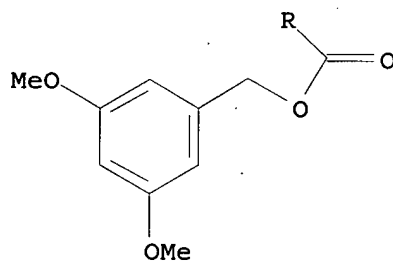
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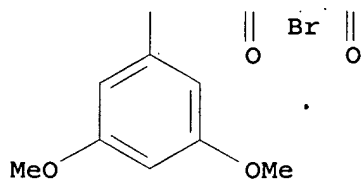
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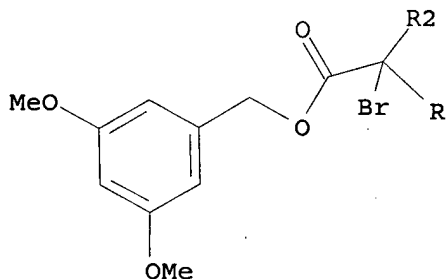
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CC 22-13 (Physical Organic Chemistry)  
 Section cross-reference(s): 25, 75

IT 681846-24-2  
 RL: PRP (Properties)  
 (crystal structure; design and synthesis of multi-component  
 18 $\pi$ -annulenic fluorofullerene ensembles suitable for  
 donor-acceptor applications)

IT 539825-95-1P 658065-04-4P 658065-05-5P  
 658065-06-6P 681846-11-7P 681846-12-8P  
 681846-13-9P 681846-14-0P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (design and synthesis of multi-component 18 $\pi$ -annulenic  
 fluorofullerene ensembles suitable for donor-acceptor  
 applications)

IT 68128-93-8P 475290-45-0P 539825-96-2P 658065-23-7P  
 681846-16-2P 681846-21-9P 681846-22-0P  
 681846-23-1P 681853-89-4P 681853-90-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (design and synthesis of multi-component 18 $\pi$ -annulenic  
 fluorofullerene ensembles suitable for donor-acceptor  
 applications)

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE  
 FOR THIS RECORD. ALL CITATIONS AVAILABLE  
 IN THE RE FORMAT

L12 ANSWER 13 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:958549 HCAPLUS

DOCUMENT NUMBER: 140:235484

TITLE: Reaction of [60]fullerene with free radicals  
 generated from active methylene compounds by  
 manganese(III) acetate dihydrate

AUTHOR(S): Zhang, Ting-Hu; Lu, Ping; Wang, Fan; Wang,  
 Guan-Wu

CORPORATE SOURCE: Department of Chemistry, University of Science

and Technology of China, Hefei, 230026, Peop.  
Rep. China

SOURCE: Organic & Biomolecular Chemistry (2003), 1(24),  
4403-4407  
CODEN: OBCRAK; ISSN: 1477-0520

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:235484

AB The reaction of [60]fullerene with di-Me malonate and di-Et malonate  
in the presence of manganese(III) acetate dihydrate  
[Mn(OAc)3·2H2O] for 20 min afforded singly bonded  
[60]fullerene dimers in a 1,4-addition pattern. When the reaction time  
was extended to 1 h, 1,4-bisadducts were obtained. An unsym.  
1,4-adduct and a C2 sym. 1,16-bisadduct were obtained when di-Et  
bromomalonate was used as the active methylene compound. Reaction of  
[60]fullerene with malononitrile and Et cyanoacetate with the aid of  
Mn(OAc)3·2H2O produced methanofullerenes. It is proposed  
that all these products were formed via the addition of free radicals  
from the active methylene compds. generated by Mn(OAc)3·2H2O.

IT 666837-07-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
RACT (Reactant or reagent)  
(reaction of [60]fullerene with free radicals generated from  
active methylene compds. by manganese(III) acetate dihydrate)

RN 666837-07-6 HCAPLUS

CN [1,1' (7H,7'H) -Bi[5,6]fullerene-C60-Ih] -7,7'-diacetic acid,  
α,α'-bis(methoxycarbonyl)-, dimethyl ester,  
(1R,1'S,7R,7'S) - (9CI) (CA INDEX NAME)

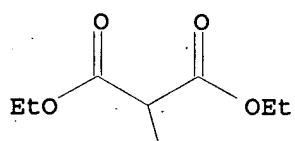
\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

IT 573951-18-5P 666837-10-1P 666837-12-3P  
666837-15-6P 666837-17-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(reaction of [60]fullerene with free radicals generated from  
active methylene compds. by manganese(III) acetate dihydrate)

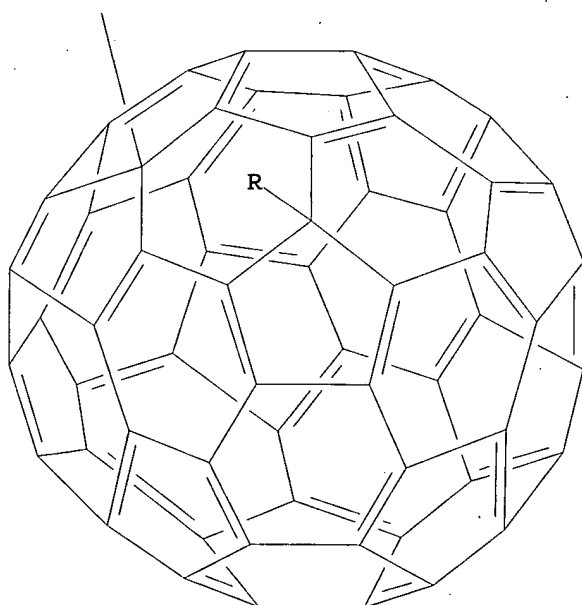
RN 573951-18-5 HCAPLUS

CN [5,6]Fullerene-C60-Ih-1,7-diacetic acid, α,α'-  
bis(ethoxycarbonyl)-, diethyl ester (9CI) (CA INDEX NAME)

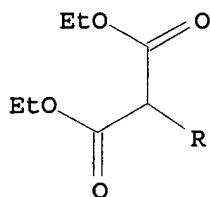
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PAGE 3-A

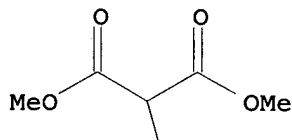


RN 666837-10-1 HCAPLUS  
CN [1,1' (7H,7'H)-Bi[5,6]fullerene-C60-Ih]-7,7'-diacetic acid,  
 $\alpha,\alpha'$ -bis(ethoxycarbonyl)-, diethyl ester,  
(1R,1'S,7R,7'S)- (9CI) (CA INDEX NAME)

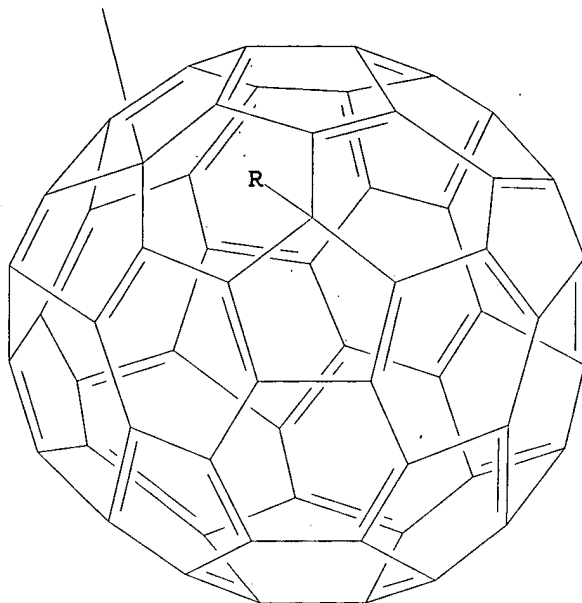
\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 666837-12-3 HCAPLUS  
CN [5,6]Fullerene-C60-Ih-1,7-diacetic acid,  $\alpha,\alpha'$ -  
bis(methoxycarbonyl)-, dimethyl ester (9CI) (CA INDEX NAME)

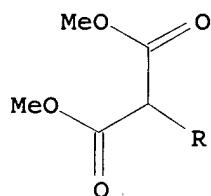
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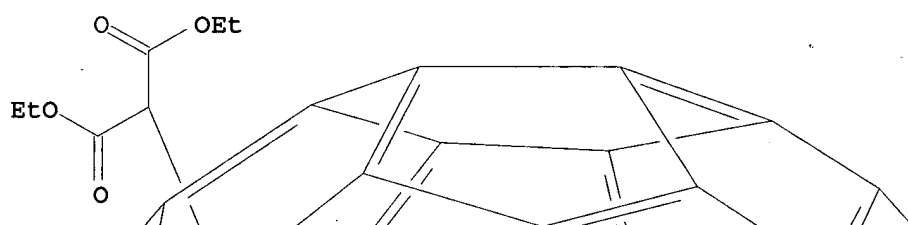
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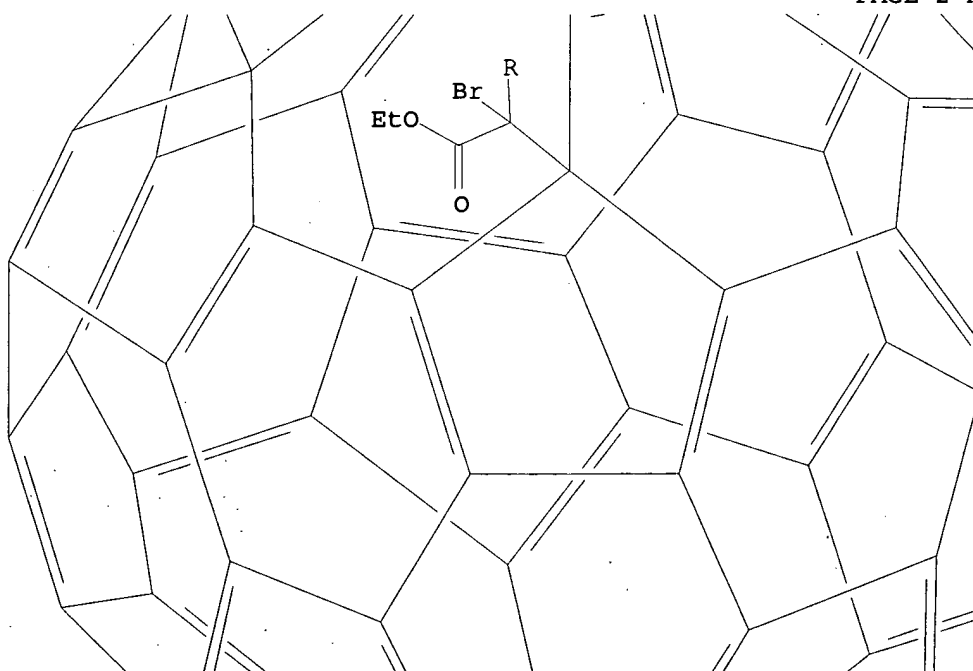
RN 666837-15-6 HCAPLUS  
CN [5,6]Fullerene-C60-1h-1,7-diacetic acid,  $\alpha$ -bromo-  
 $\alpha,\alpha'$ -bis(ethoxycarbonyl)-, diethyl ester (9CI) (CA  
INDEX NAME)



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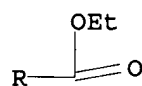
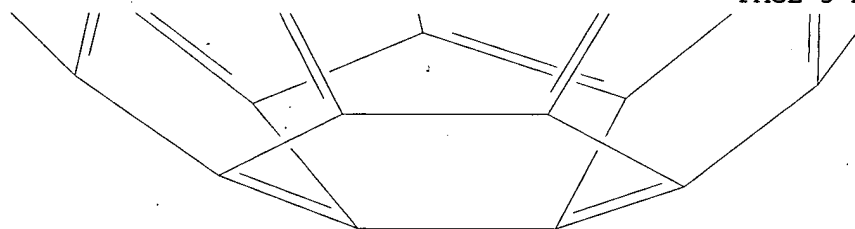
PAGE 2-A



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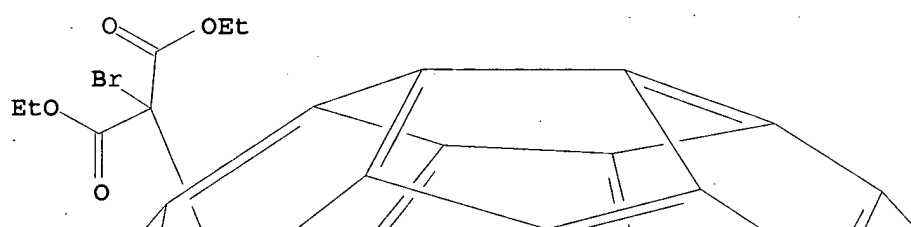
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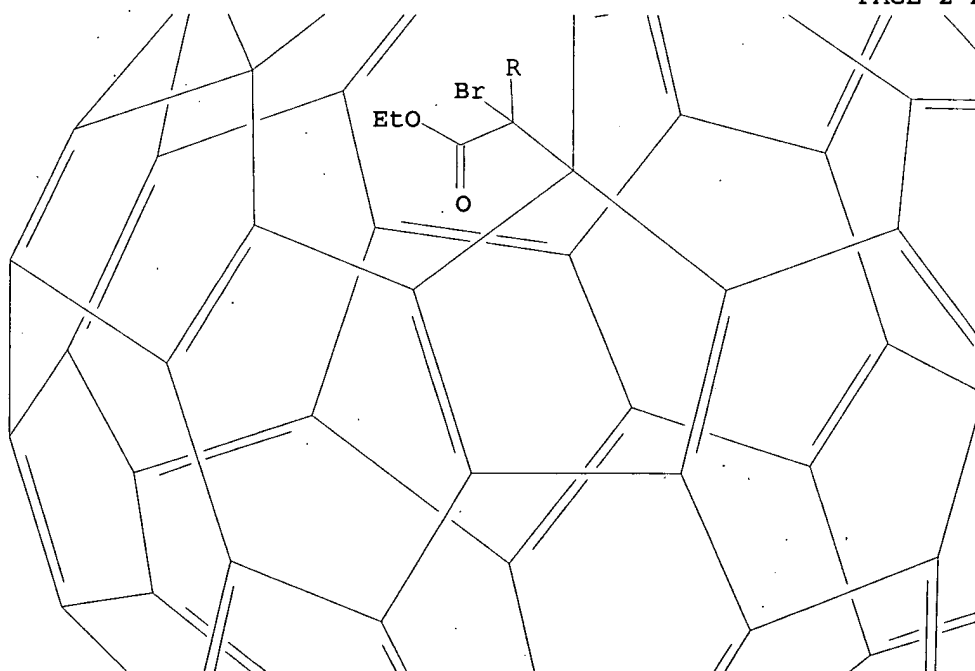
PAGE 3-B

RN 666837-17-8 HCAPLUS  
 CN [5,6]Fullerene-C60-1h-1,7-diacetic acid,  $\alpha,\alpha'$ -dibromo-  
 $\alpha,\alpha'$ -bis(ethoxycarbonyl)-, diethyl ester (9CI) (CA  
 INDEX NAME)

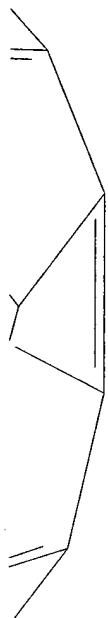
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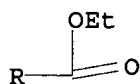
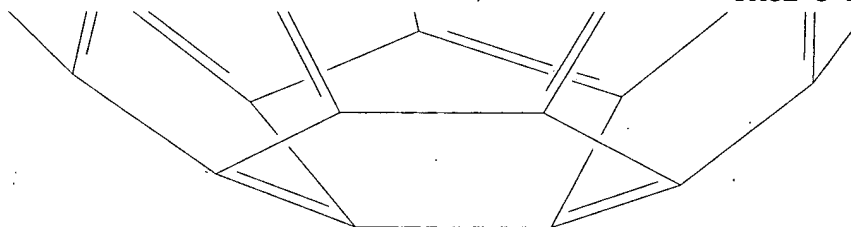
PAGE 2-A



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PAGE 3-B

CC 25-29 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
IT 666837-07-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
RACT (Reactant or reagent)  
(reaction of [60]fullerene with free radicals generated from  
active methylene compds. by manganese(III) acetate dihydrate)  
IT 176961-88-9P 176961-89-0P 573951-18-5P

666837-10-1P 666837-12-3P 666837-15-6P  
666837-17-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(reaction of [60]fullerene with free radicals generated from  
active methylene compds. by manganese(III) acetate dihydrate)

REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE  
FOR THIS RECORD. ALL CITATIONS AVAILABLE  
IN THE RE FORMAT

L12 ANSWER 14 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:683506 HCAPLUS

DOCUMENT NUMBER: 140:181198

TITLE: Synthesis and characterisation of trannulated  
fluorofullerenes: A new generation of  
donor-acceptor materials

AUTHOR(S): Burley, Glenn A.; Avent, Anthony G.; Boltalina,  
Olga G.; Gol'dt, Ilya V.; Kuvytchko, Igor;  
Pascuale, Federico; Taylor, Roger

CORPORATE SOURCE: School of Chemistry, Physics and Environmental  
Sciences, University of Sussex, Brighton, BN1  
9QJ, UK

SOURCE: Proceedings - Electrochemical Society (2002),  
2002-12(Fullerenes--Volume 12: The Exciting  
World of Nanocages and Nanotubes), 225-233  
CODEN: PESODO; ISSN: 0161-6374

PUBLISHER: Electrochemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:181198

AB A variety of trannulated (all trans annulated) fluorofullerene  
derivs. were prepared by a simple 1-step addition of substituted di-Et  
methanetricarboxylate anions to C<sub>60</sub>F<sub>18</sub>. This reaction provides an  
efficient synthetic route to multi-component donor-acceptor systems  
for potential photovoltaic applications. <sup>1</sup>H and <sup>19</sup>F NMR  
spectroscopy revealed restricted rotation around the carbon-carbon  
bond connecting the addend with the fullerene core. The presence of  
conformational isomerism in these trannulated fluorofullerene  
derivs. was found to vary with increasing steric bulk of the  
addends.

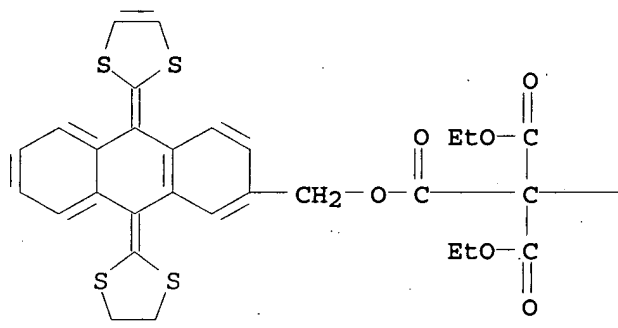
IT 539825-95-1P 539825-96-2P 658065-04-4P  
658065-05-5P 658065-06-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of trans annulated fluorofullerenes)

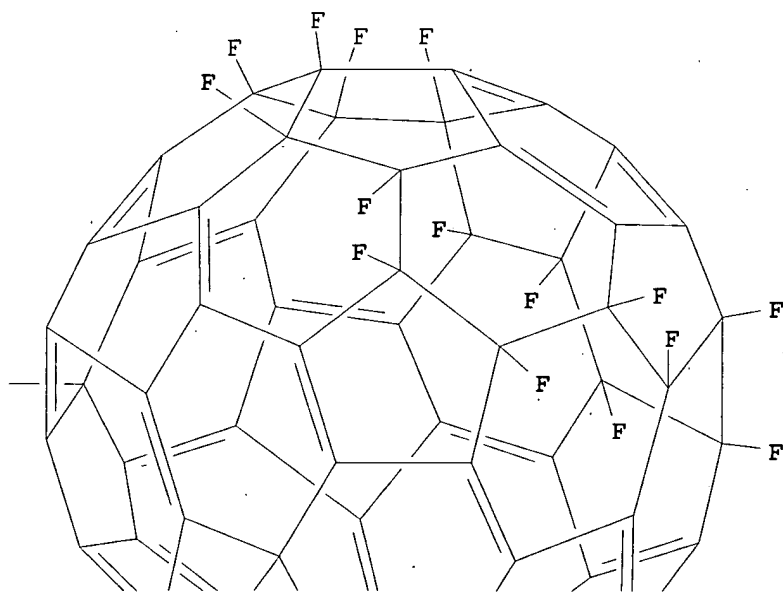
RN 539825-95-1 HCAPLUS

CN [5,6]Fullerene-C<sub>60</sub>-1h-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha,\alpha',\alpha',\alpha'',\alpha''$ -  
hexakis(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
tetradecahydro-, tris[[9,10-bis(1,3-dithiol-2-ylidene)-9,10-dihydro-  
2-anthracenyl]methyl] ester (9CI) (CA INDEX NAME)

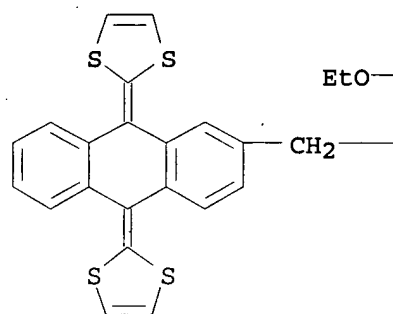
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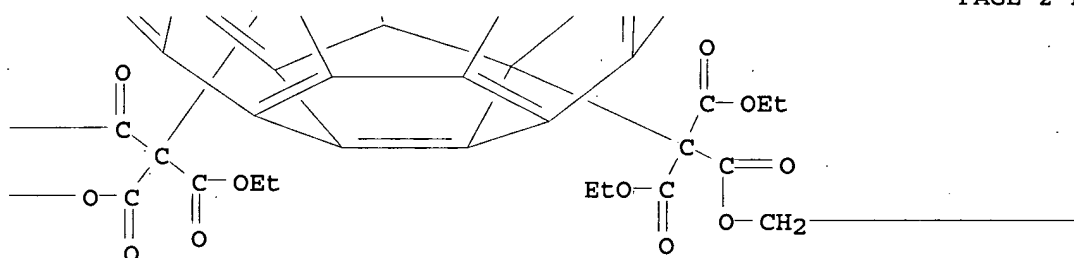
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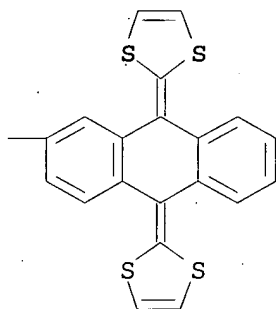
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PAGE 2-B

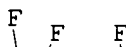


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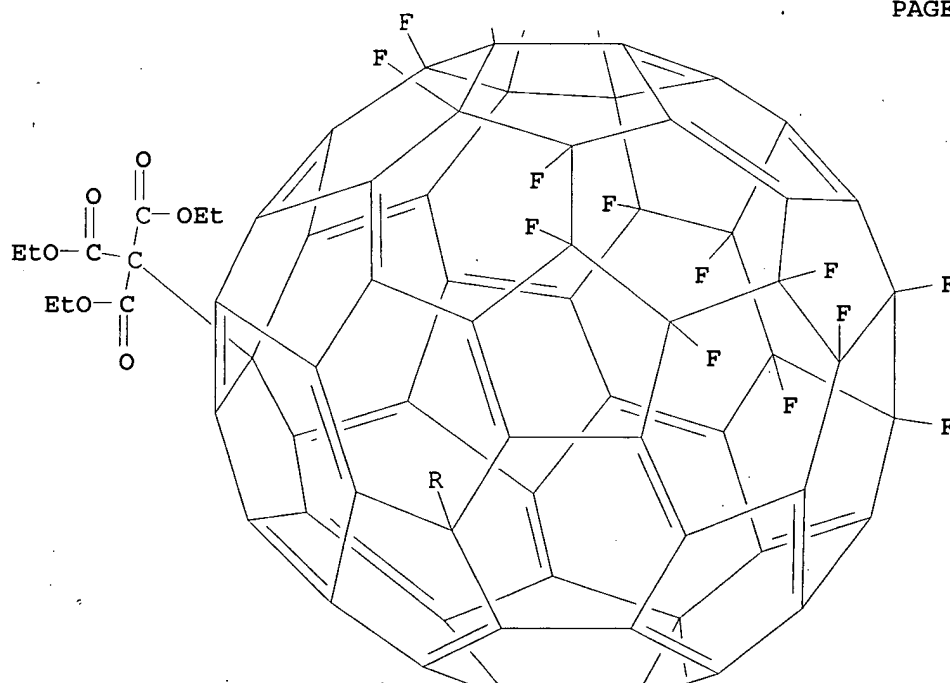


RN 539825-96-2 HCAPLUS  
 CN [5,6]Fullerene-C60-1h-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha,\alpha',\alpha',\alpha'',\alpha''$ -  
 hexakis(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 tetradecahydro-, triethyl ester (9CI) (CA INDEX NAME)

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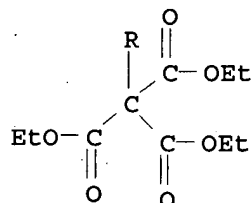
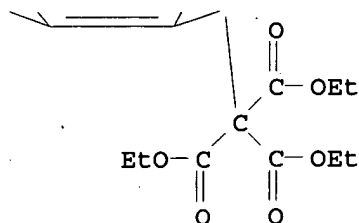


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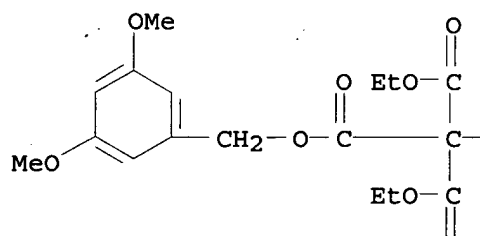


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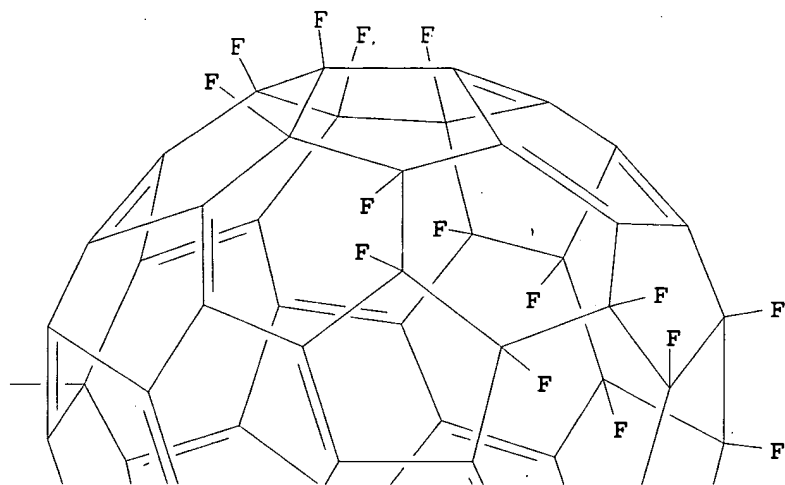


RN 658065-04-4 HCAPLUS  
 CN [5,6]Fullerene-C60-1h-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha,\alpha',\alpha',\alpha'',\alpha''$ -  
 hexakis(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 tetradecahydro-, tris[(3,5-dimethylphenyl)methyl] ester (9CI) (CA  
 INDEX NAME)

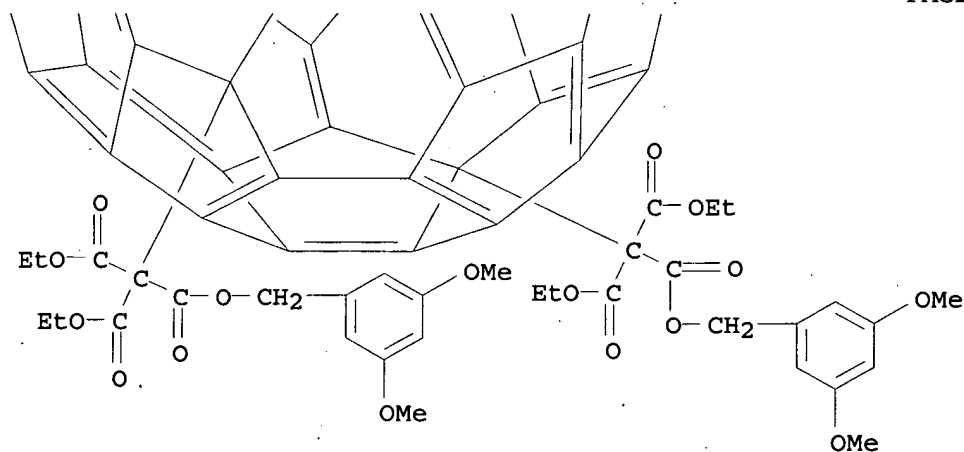
PAGE 1-A



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PAGE 2-A  
O

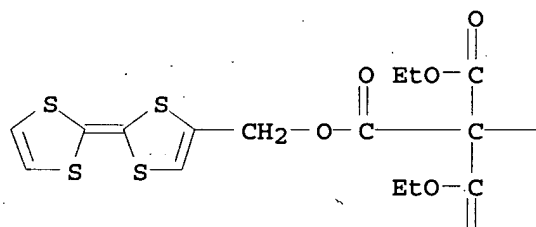
PAGE 2-B



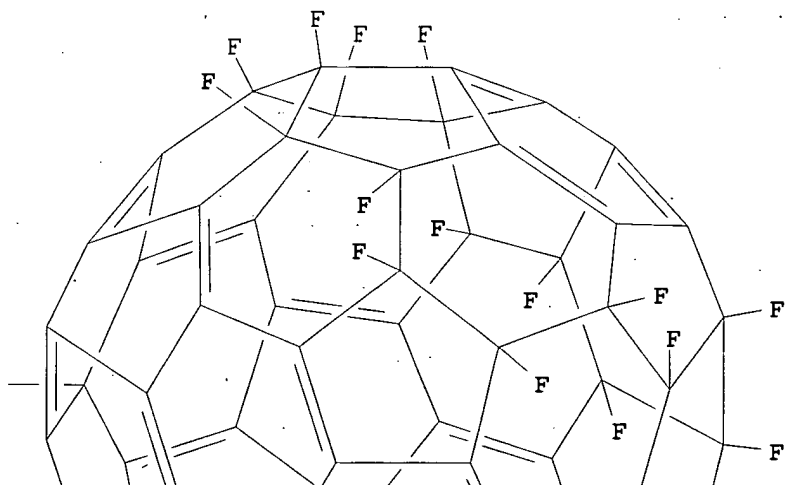
RN 658065-05-5 HCAPLUS  
 CN [5,6]Fullerene-C60-1h-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha,\alpha',\alpha',\alpha'',\alpha''$ -  
 hexakis(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 tetradecahydro-, tris[[2-(1,3-dithiol-2-ylidene)-1,3-dithiol-4-

yl)methyl] ester (9CI) (CA INDEX NAME)

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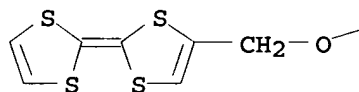
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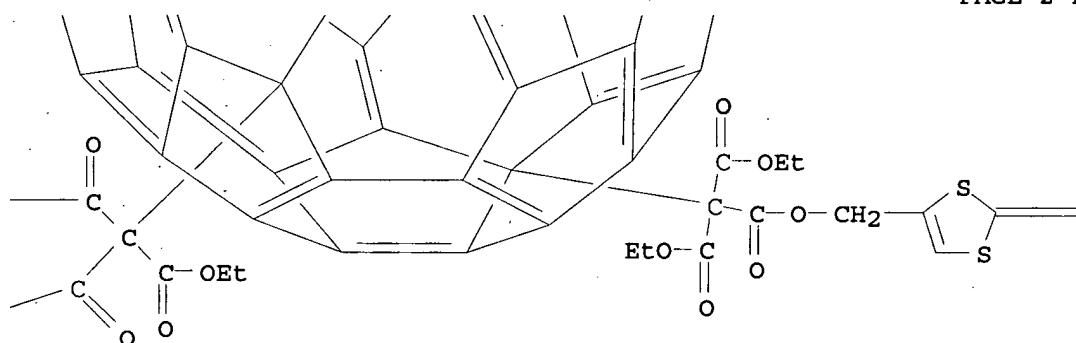
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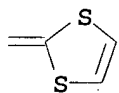
EtO—



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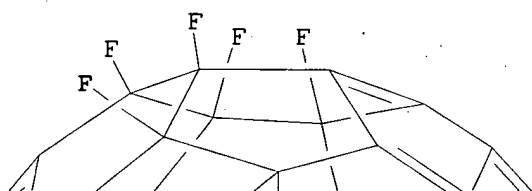


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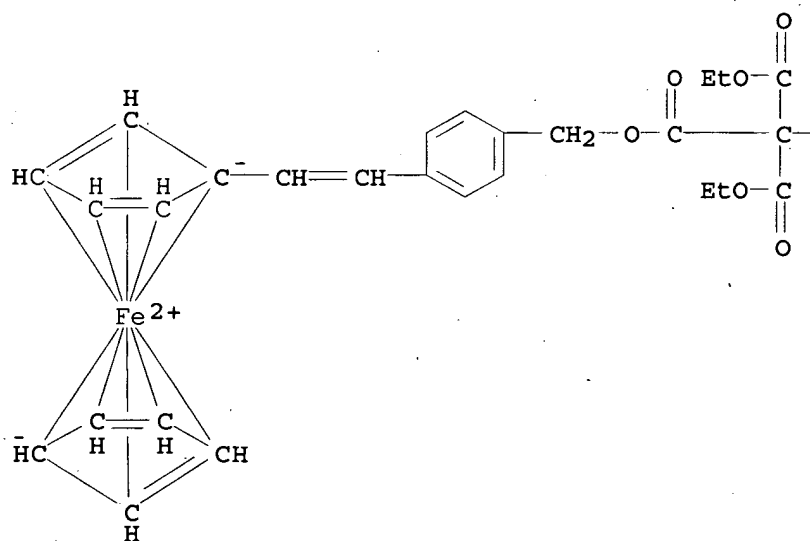


RN 658065-06-6 HCAPLUS  
 CN Ferrocene, 1,1',1',1'-[(23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-tetradecahydro[5,6]fullerene-C60-1h-1,33,38(23H)-triyl)tris[[2,2-bis(ethoxycarbonyl)-1-oxo-2,1-ethanediyl]oxymethylene-4,1-phenylene-2,1-ethenediyl]]tris- (9CI) (CA INDEX NAME)

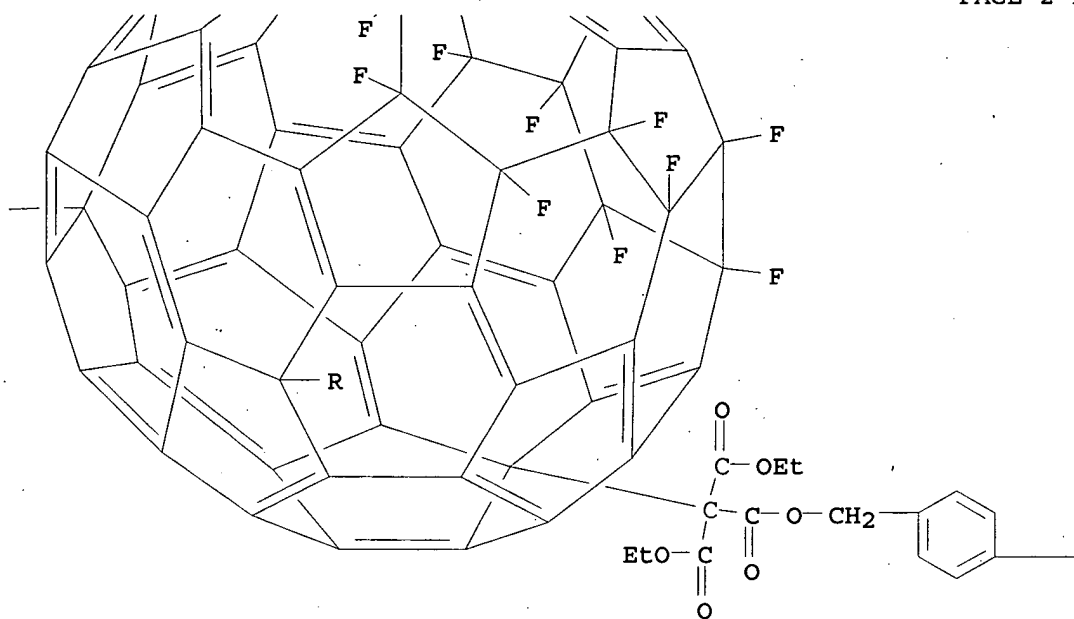
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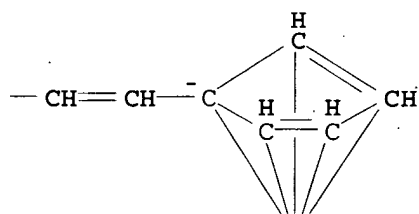
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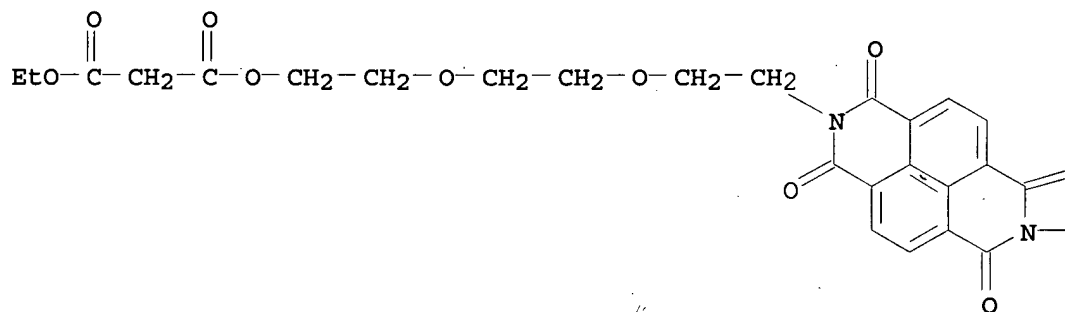
The chemical structure shows a ferrocene molecule, which consists of two cyclopentadienyl rings sandwiching an iron atom in the  $\text{Fe}^{2+}$  oxidation state. The top cyclopentadienyl ring is substituted with a side chain at the 1-position:  $-\text{CH}=\text{CH}-\text{C}(=\text{O})-\text{O}-\text{CH}_2-\text{C}_6\text{H}_4-\text{C}(=\text{O})-\text{O}-\text{C}(=\text{O})-\text{R}$ . The bottom cyclopentadienyl ring is substituted with a methyl group ( $-\text{CH}_3$ ) at the 1-position. The side chain includes an ester group, a benzene ring, and a ketone group.

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of trans annulated fluorofullerenes)

03/31/2008

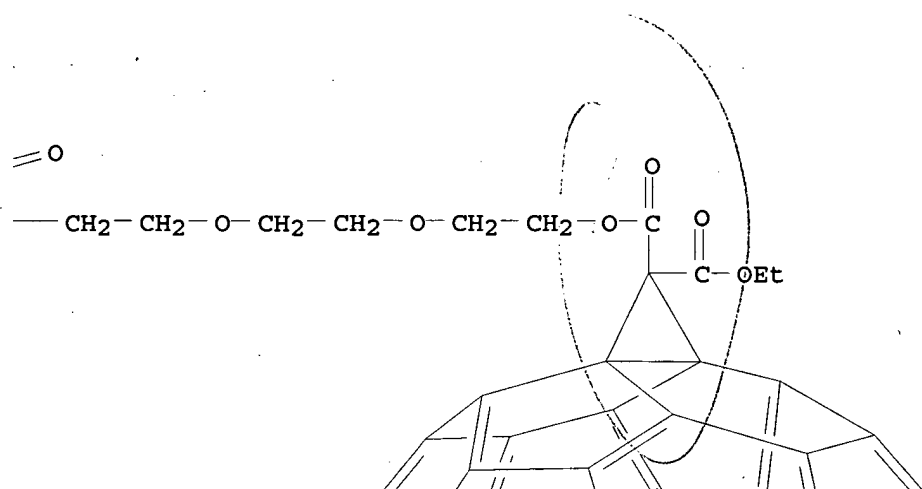
SOURCE: Angewandte Chemie, International Edition (2003),  
42(27), 3158-3162  
CODEN: ACIEF5; ISSN: 1433-7851  
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 139:276625  
AB Intramol. Bingel reaction of monoadducts 3a and 3b in the presence  
of 1,5-dinaphtho-[38]-crown-10-ether 4 afforded at -78 °C  
novel neutral [2]catenanes 1a and 1b, while the intermol. Bingel  
reaction of 3a and 3b with [60]fullerene gave [2]rotaxanes 2a and  
2b.  
IT 606143-08-2P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP  
(Preparation)  
([2]catenane; preparation of neutral [60]fullerene-based [2]catenanes  
and [2]rotaxanes bearing electron-deficient aromatic diimide moiety)  
RN 606143-08-2 HCAPLUS  
CN 3'H-Cyclopropa[1,9][5,6]fullerene-C60-Ih-3',3'-dicarboxylic acid,  
2-[2-[2-[7-(10,12-dioxo-3,6,9,13-tetraoxapentadec-1-yl)-3,6,7,8-  
tetrahydro-1,3,6,8-tetraoxobenzo[lmn][3,8]phenanthrolin-2(1H)-  
yl]ethoxy]ethoxy]ethyl ethyl ester, rotaxane compd. with  
6,9,12,15,18,29,32,35,38,41-decaoxapentacyclo[40.4.0.05,46.019,24.02  
3,28]hexatetraconta-1,3,5(46),19,21,23,25,27,42,44-decaene (1:1)  
(9CI) (CA INDEX NAME)  
CM 1  
CRN 606143-07-1  
CMF C96 H40 N2 O16

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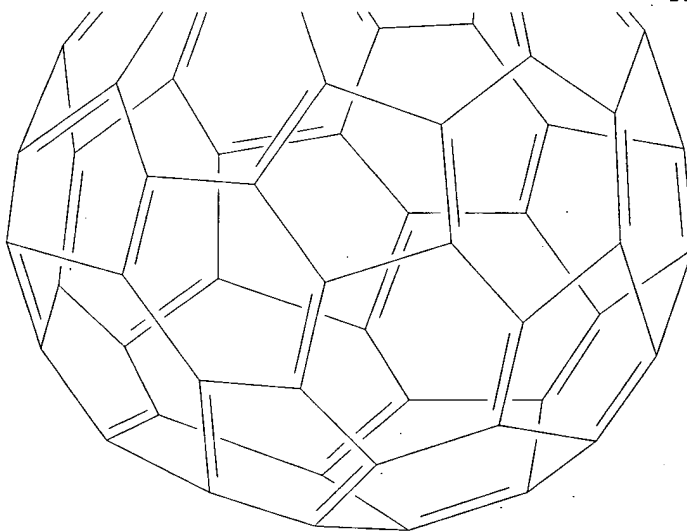




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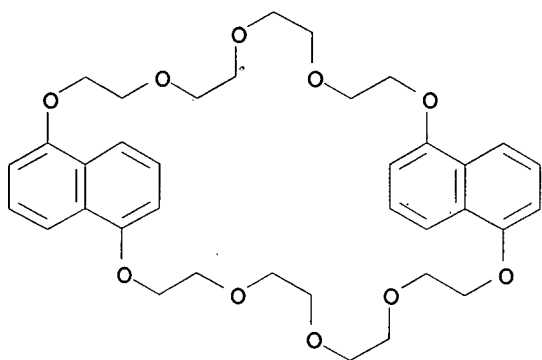
PAGE 2-B



CM 2

CRN 116059-04-2

CMF C36 H44 O10



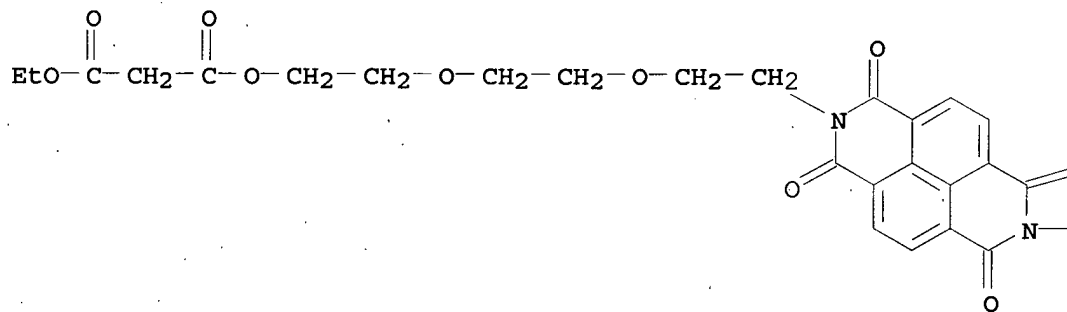
IT 606143-07-1

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of neutral [60]fullerene-based [2]catenanes and  
 [2]rotaxanes bearing electron-deficient aromatic diimide moiety)

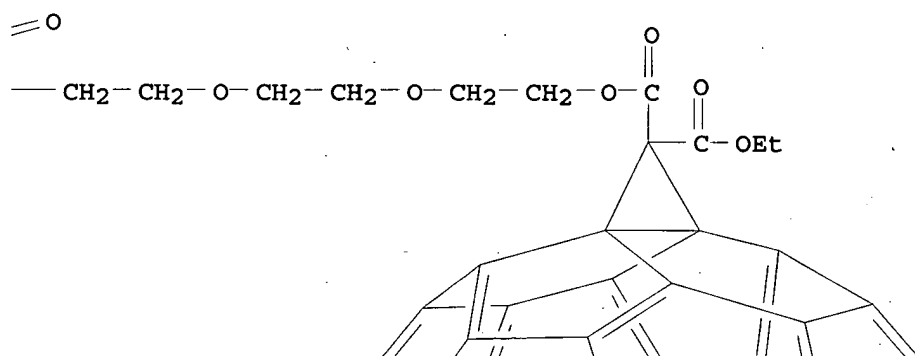
RN 606143-07-1 HCAPLUS

CN 3'H-Cyclopropa[1,9][5,6]fullerene-C60-Ih-3',3'-dicarboxylic acid,  
 2-[2-[2-[7-(10,12-dioxo-3,6,9,13-tetraoxapentadec-1-yl)-3,6,7,8-  
 tetrahydro-1,3,6,8-tetraoxobenzo[lmn][3,8]phenanthroline-2(1H)-  
 yl]ethoxy]ethoxy]ethyl ethyl ester (9CI) (CA INDEX NAME)

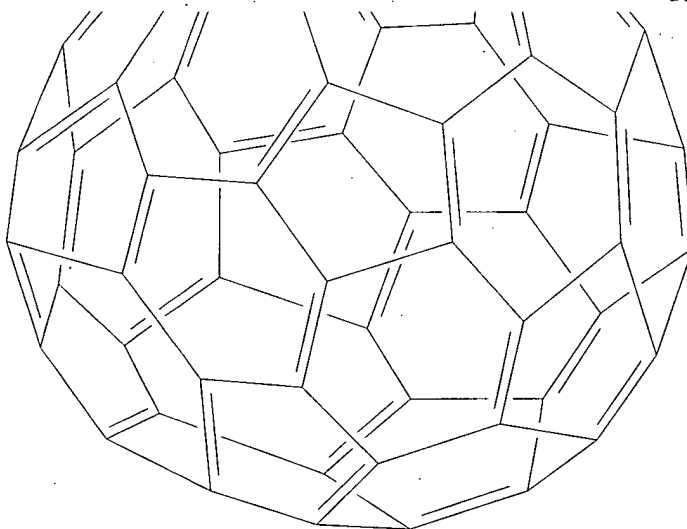
PAGE 1-A



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IT 606143-12-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(preparation of neutral [60]fullerene-based [2]catenanes and [2]rotaxanes bearing electron-deficient aromatic diimide moiety)

RN 606143-12-8 HCAPLUS

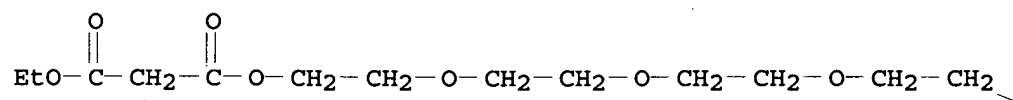
CN 3'H-Cyclopropa[1,9][5,6]fullerene-C60-1h-3',3'-dicarboxylic acid,  
2-[2-[2-[2-[7-(13,15-dioxo-3,6,9,12,16-pentaoxaoctadec-1-yl)-3,6,7,8-

CM 1

CRN 606143-11-7

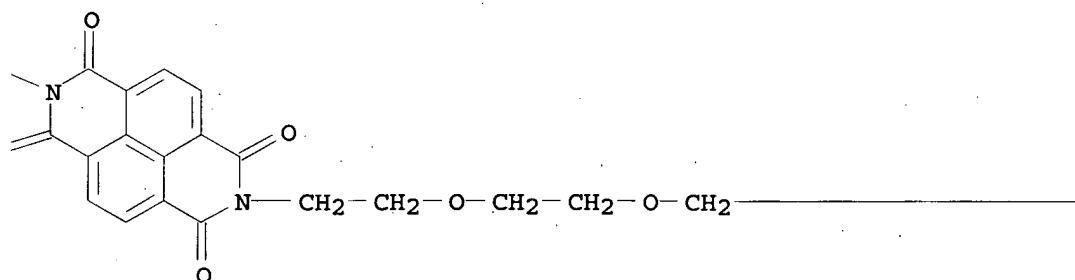
CMF C100 H48 N2 O18

PAGE 1-A

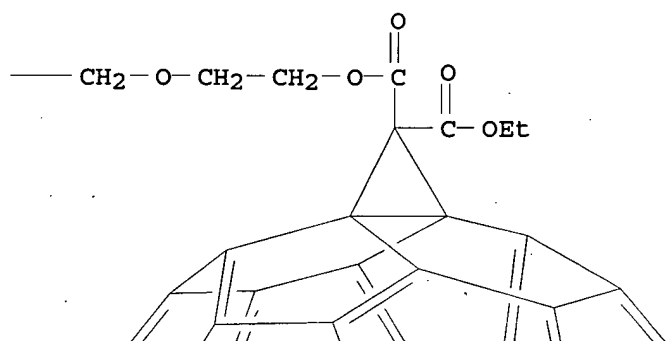


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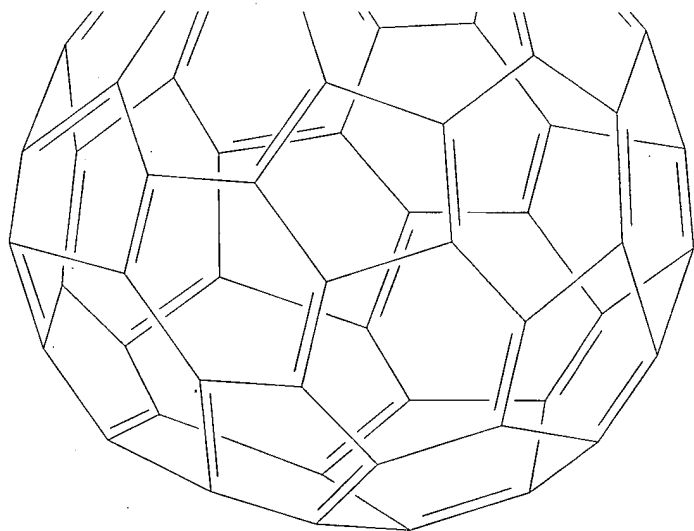
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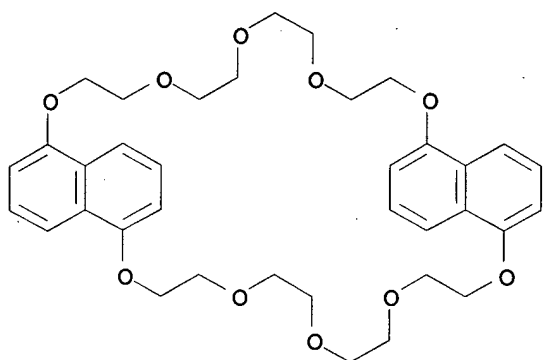
PAGE 2-C



CM 2

CRN 116059-04-2

CMF C36 H44 O10



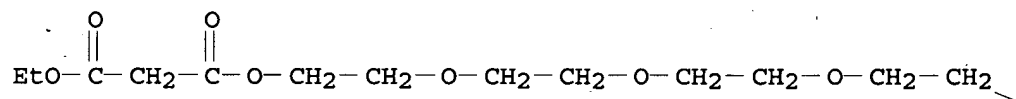
IT 606143-11-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of neutral [60]fullerene-based [2]catenanes and  
 [2]rotaxanes bearing electron-deficient aromatic diimide moiety)

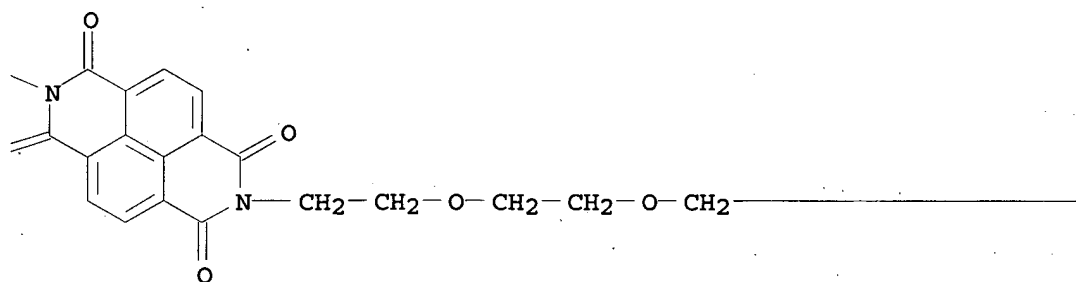
RN 606143-11-7 HCAPLUS

CN 3'H-Cyclopropa[1,9][5,6]fullerene-C60-1h-3',3'-dicarboxylic acid,  
 2-[2-[2-[2-[7-(13,15-dioxo-3,6,9,12,16-pentaoxaoctadec-1-yl)-3,6,7,8-  
 tetrahydro-1,3,6,8-tetraoxobenzo[1mn][3,8]phenanthroline-2(1H)-  
 yl]ethoxy]ethoxy]ethoxy]ethyl ethyl ester (9CI) (CA INDEX NAME)

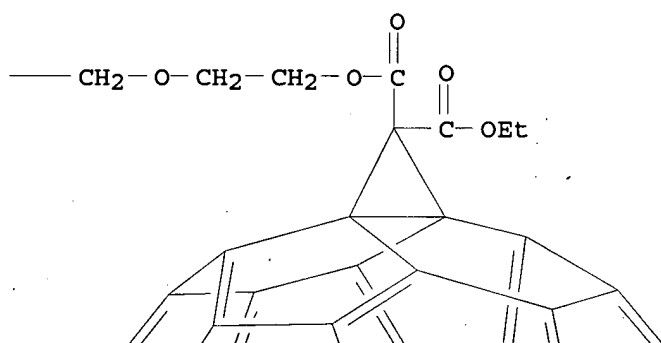
PAGE 1-A



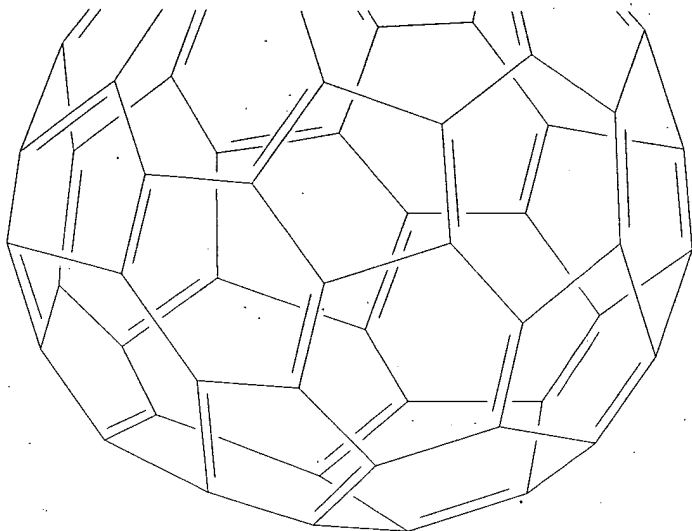
PAGE 1-B



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PAGE 2-C



CC 22-13 (Physical Organic Chemistry)  
Section cross-reference(s): 28

IT 606143-08-2P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
([2]catenane; preparation of neutral [60]fullerene-based [2]catenanes and [2]rotaxanes bearing electron-deficient aromatic diimide moiety)

IT 116059-04-2 606143-07-1  
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)  
(preparation of neutral [60]fullerene-based [2]catenanes and [2]rotaxanes bearing electron-deficient aromatic diimide moiety)

IT 606143-12-8P 606143-14-0P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation of neutral [60]fullerene-based [2]catenanes and [2]rotaxanes bearing electron-deficient aromatic diimide moiety)

IT 99685-96-8, C60 Fullerene 606143-11-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of neutral [60]fullerene-based [2]catenanes and [2]rotaxanes bearing electron-deficient aromatic diimide moiety)

REFERENCE COUNT: 68 THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 16 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2003:491972 HCAPLUS  
DOCUMENT NUMBER: 139:230217  
TITLE: Synthesis of  $18\pi$  annulenic fluorofullerenes from tertiary carbanions: size matters  
AUTHOR(S): Burley, Glenn A.; Avent, Anthony G.; Boltalina, Olga V.; Drewello, Thomas; Goldt, Ilya V.; Marcaccio, Massimo; Paolucci, Francesco; Paolucci, Demis; Street, Joan M.; Taylor, Roger  
CORPORATE SOURCE: School of Chemistry, Physics and Environmental Sciences, University of Sussex, Brighton, BN1 9QJ, UK  
SOURCE: Organic & Biomolecular Chemistry (2003), 1(11),



2015-2023

CODEN: OBCRAK; ISSN: 1477-0520

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:230217

AB A range of tertiary carbanions  $XCH(CO_2Et)_2$  of differing sizes have been reacted with  $C_{60}F_{18}$  to assess the steric effect of X on the position of nucleophilic substitution. For X =  $CO_2Et$ ,  $NO_2$ ,  $P(O)(OMe)_2$ ,  $SO_2CH_2Ph$ , the all trans annulenes (trannulenes) were obtained as a result of extended  $SN_2'$  (i.e.  $SN_2''$ ) substitution; in the case of the phosphorus compound, with reduced amts. of base (DBU) dephosphonylation of one or more  $P(O)(OMe)_2$  groups by hydrogen occurred. Trannulene formation did not occur for X = F, CN due to the smaller size of the nucleophile, and in the latter case substitution was shown to take place by an  $SN_2'$  mechanism, resulting in the addend being adjacent to a fluorine addend. Trannulenes (X =  $CO_2Et$ , Br, Cl) exhibited reversible one-electron redns. at potentials (-0.02 to -0.09 V) significantly more pos. than for [60]fullerene. Trannulene (X =  $NO_2$ ) exhibited an irreversible one-electron reduction (0.08 V); the irreversibility may be associated with fluorine loss. Conformational isomerism at temps. below 298 K was observed for all trannulene derivs. as a result of eclipsing addend-addend interactions. Min. energy conformations with a rotational energy barrier of 12-15 kcal mol<sup>-1</sup> were observed when these interactions are calculated using mol. mechanics.

IT 591722-01-9 591722-02-0

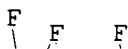
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(UV-Vis-NIR spectrum; steric effect on synthesis of  $18\pi$  annulenic fluorofullerenes by nucleophilic substitution reaction of tertiary carbanions with  $C_{60}F_{18}$ )

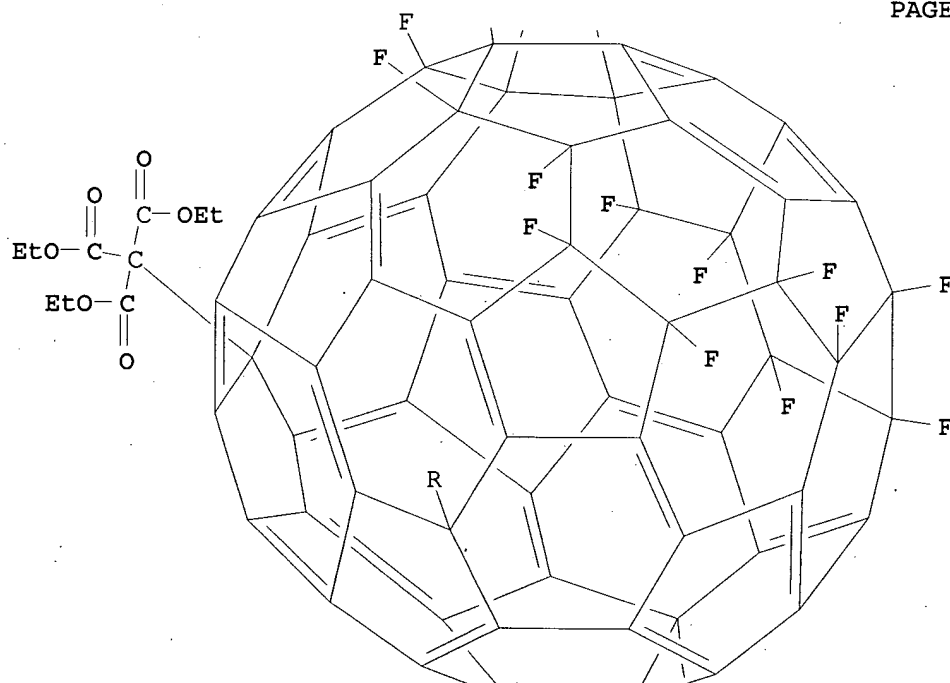
RN 591722-01-9 HCAPLUS

CN [5,6]Fullerene- $C_{60}$ -1h-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha,\alpha',\alpha',\alpha'',\alpha''$ -  
hexakis(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
tetradecahydro-, triethyl ester, radical ion(1-) (9CI) (CA INDEX  
NAME)

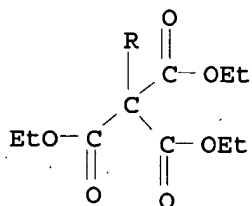
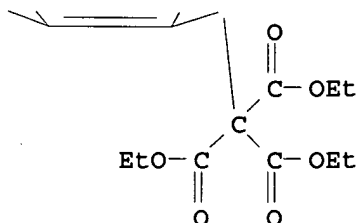
PAGE 1-A



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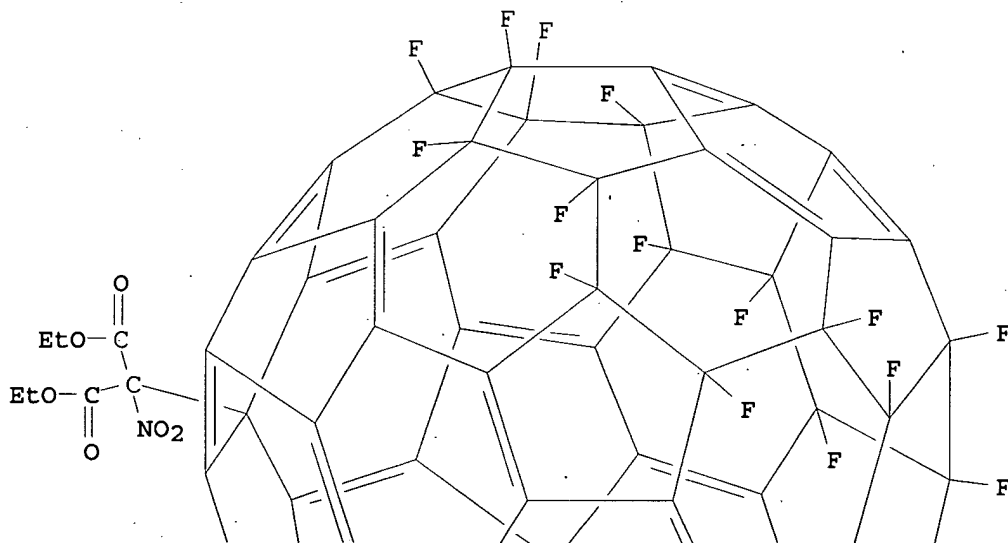


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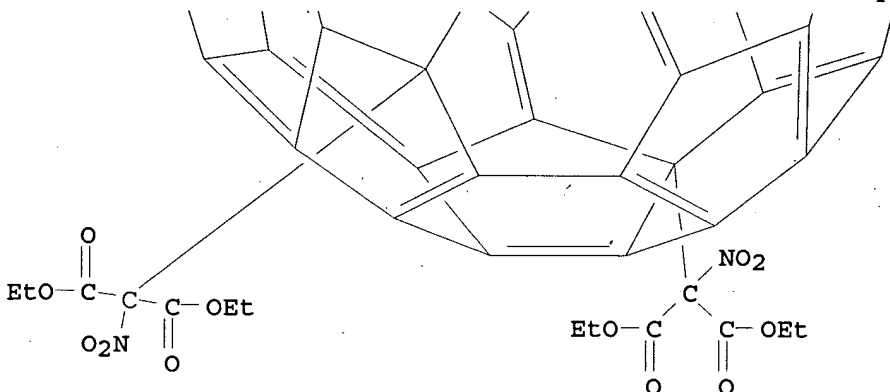


RN 591722-02-0 HCAPLUS  
 CN [5,6]Fullerene-C60-1h-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha',\alpha''$ -tris(ethoxycarbonyl)-  
 23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-pentadecafluoro-  
 24,25,26,27,28,41,42,47,48,49,55,56,59,60-tetradecahydro-  
 $\alpha,\alpha',\alpha''$ -trinitro-, triethyl ester, radical  
 ion(1-) (9CI) (CA INDEX NAME)

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IT 539825-96-2P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(electrochem. and conformational isomerism; steric effect on synthesis of  $18\pi$  annulenic fluorofullerenes by nucleophilic substitution reaction of tertiary carbanions with C<sub>60</sub>F<sub>18</sub>)

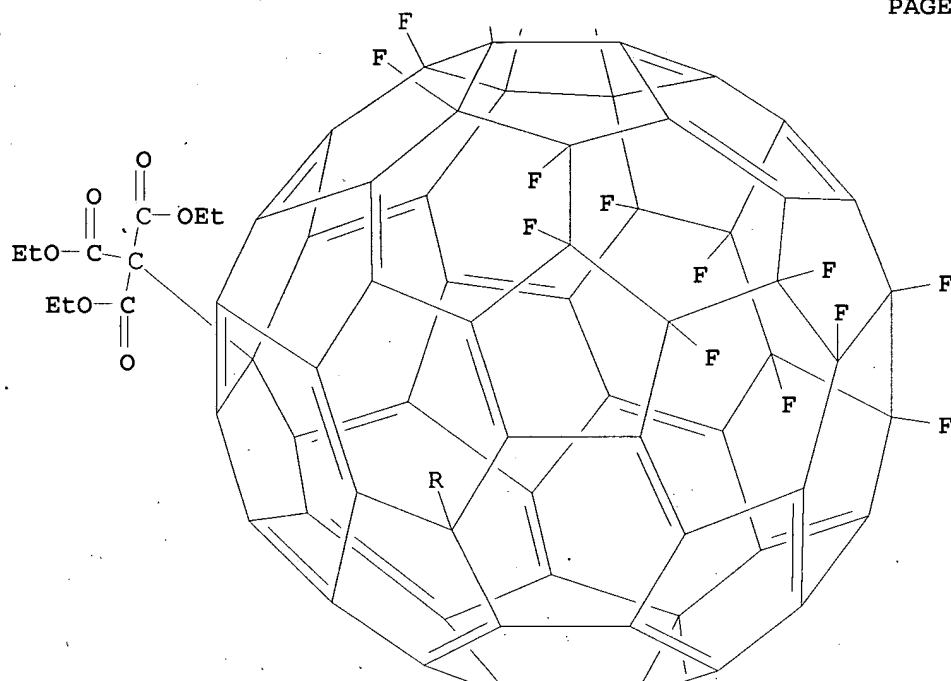
RN 539825-96-2 HCAPLUS

CN [5,6]Fullerene-C<sub>60</sub>-Ih-1,33,38(23H)-triacetic acid,  $\alpha, \alpha, \alpha', \alpha', \alpha'', \alpha''$ -hexakis(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-tetradecahydro-, triethyl ester (9CI) (CA INDEX NAME)

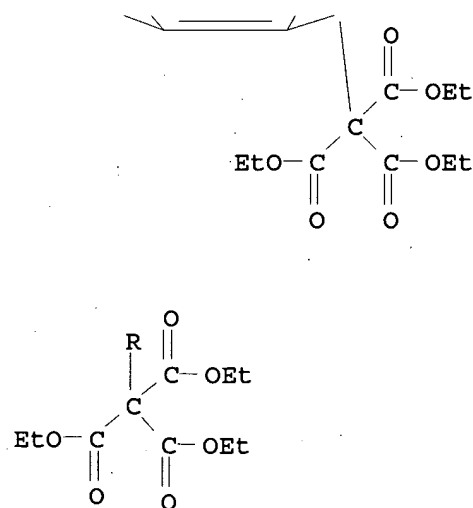
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IT 591721-96-9P

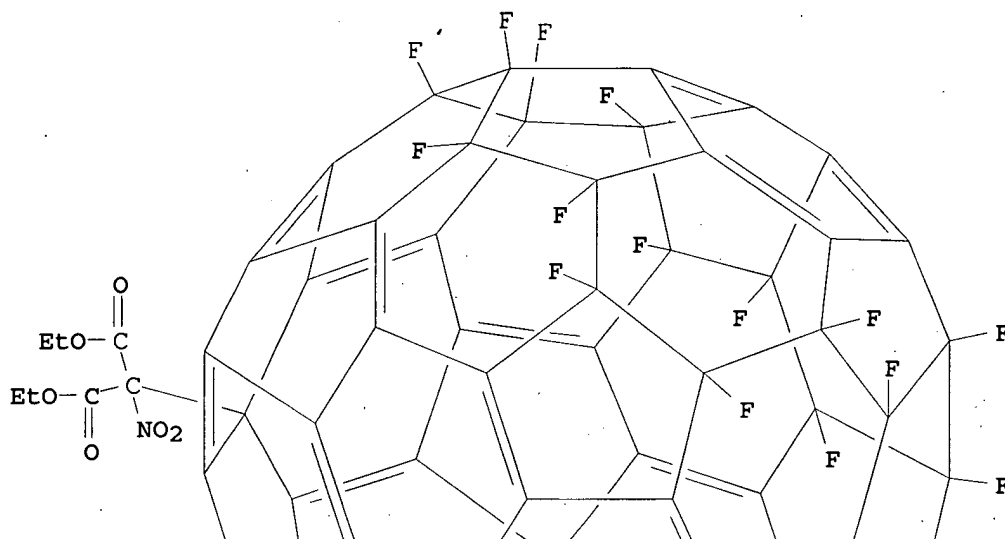
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation);  
 PREP (Preparation); RACT (Reactant or reagent)

(electrochem.; steric effect on synthesis of 18 $\pi$  annulenic  
 fluorofullerenes by nucleophilic substitution reaction of

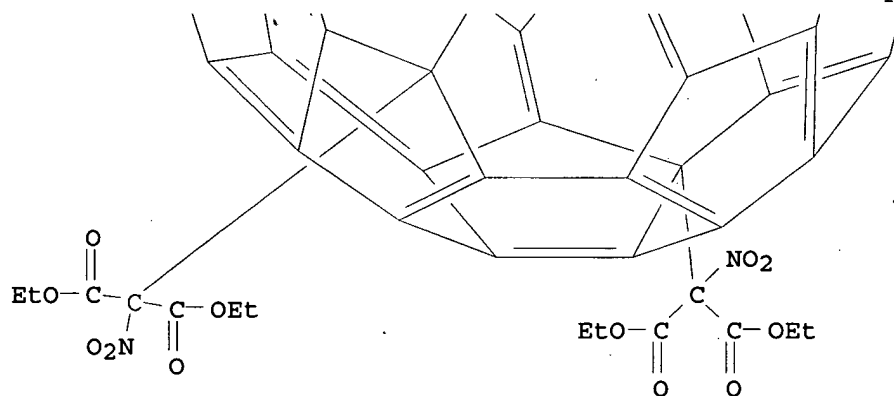
tertiary carbanions with C60F18)

RN 591721-96-9 HCAPLUS  
 CN [5,6]Fullerene-C60-Ih-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha',\alpha''$ -tris(ethoxycarbonyl)-  
 23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-pentadecafluoro-  
 24,25,26,27,28,41,42,47,48,49,55,56,59,60-tetradecahydro-  
 $\alpha,\alpha',\alpha''$ -trinitro-, triethyl ester (9CI) (CA  
 INDEX NAME)

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IT 374623-61-7 475975-88-3

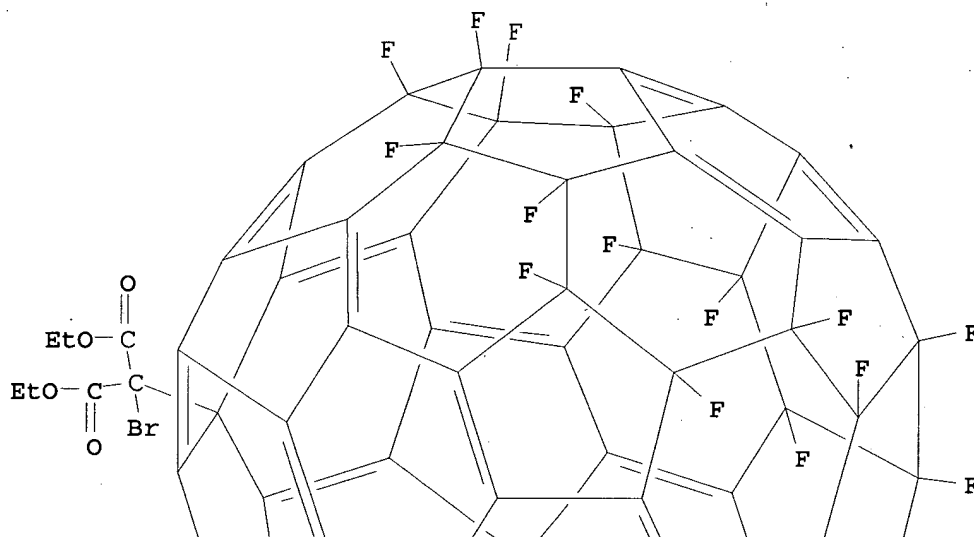
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)  
 (electronic absorption and reduction potential; steric effect on

synthesis of 18 $\pi$  annulenic fluorofullerenes by nucleophilic substitution reaction of tertiary carbanions with C<sub>60</sub>F<sub>18</sub>)

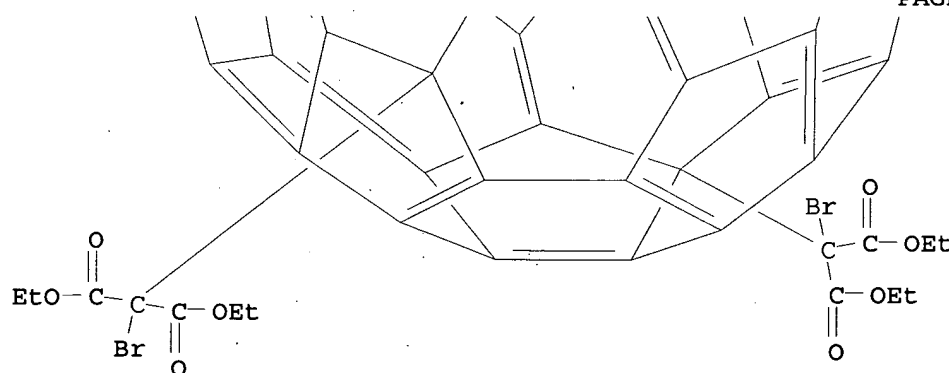
RN 374623-61-7 HCAPLUS

CN [5,6]Fullerene-C<sub>60</sub>-Ih-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha',\alpha''$ -tribromo- $\alpha,\alpha',\alpha''$ -  
 tris(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 tetradecahydro-, triethyl ester (9CI) (CA INDEX NAME)

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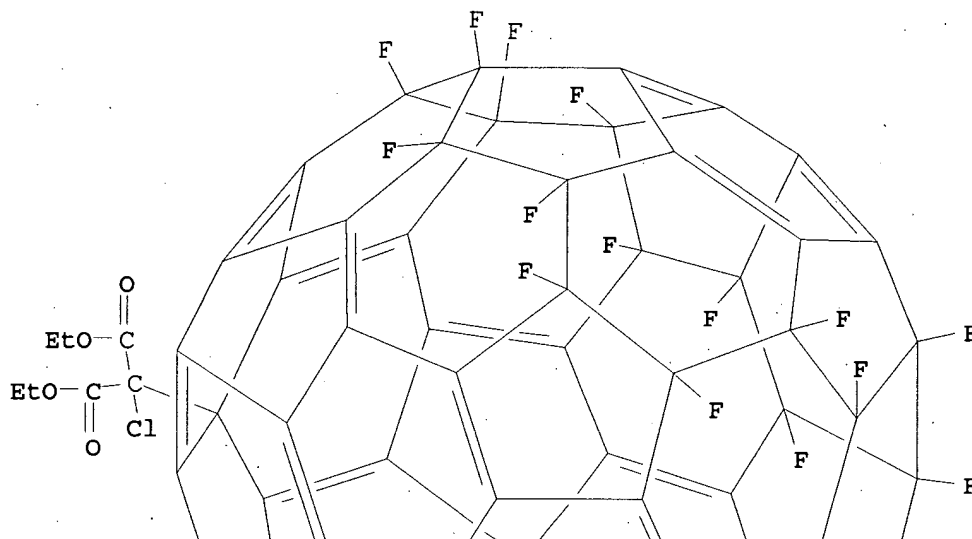


RN 475975-88-3 HCAPLUS

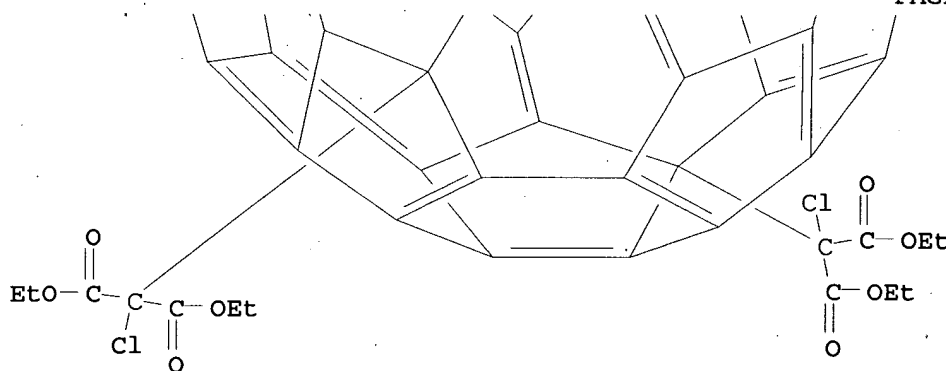
CN [5,6]Fullerene-C<sub>60</sub>-Ih-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha',\alpha''$ -trichloro- $\alpha,\alpha',\alpha''$ -  
 tris(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-

pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-tetradecahydro-, triethyl ester (9CI) (CA INDEX NAME)

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IT 591721-97-0P 591721-98-1P 591741-82-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(steric effect on synthesis of 18 $\pi$  annulenic fluorofullerenes  
by nucleophilic substitution reaction of tertiary carbanions with  
C60F18)

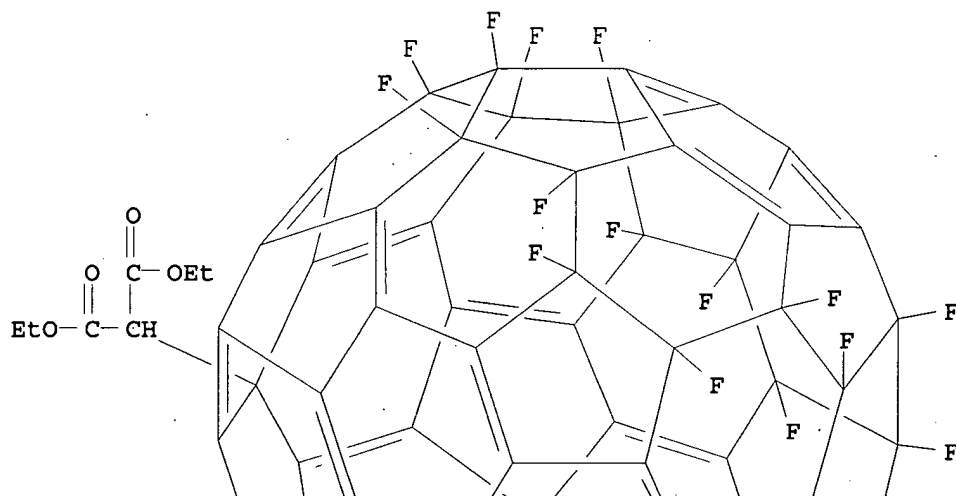
RN 591721-97-0 HCAPLUS

CN [5,6]Fullerene-C60-1h-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha',\alpha''$ -tris(ethoxycarbonyl)-  
23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-pentadecafluoro-  
24,25,26,27,28,41,42,47,48,49,55,56,59,60-tetradecahydro-, triethyl

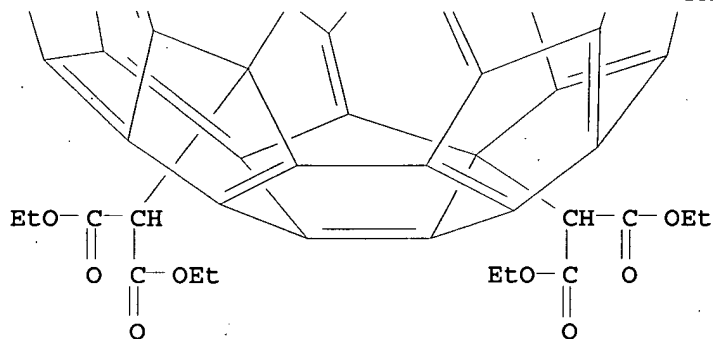


ester (9CI) (CA INDEX NAME)

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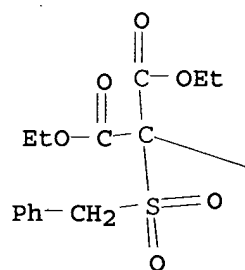


RN 591721-98-1 HCAPLUS  
 CN [5,6]Fullerene-C60-1h-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha',\alpha''$ -tris(ethoxycarbonyl)-  
 23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-pentadecafluoro-  
 24,25,26,27,28,41,42,47,48,49,55,56,59,60-tetradecahydro-  
 $\alpha,\alpha',\alpha''$ -tris[(phenylmethyl)sulfonyl]-, triethyl  
 ester (9CI) (CA INDEX NAME)

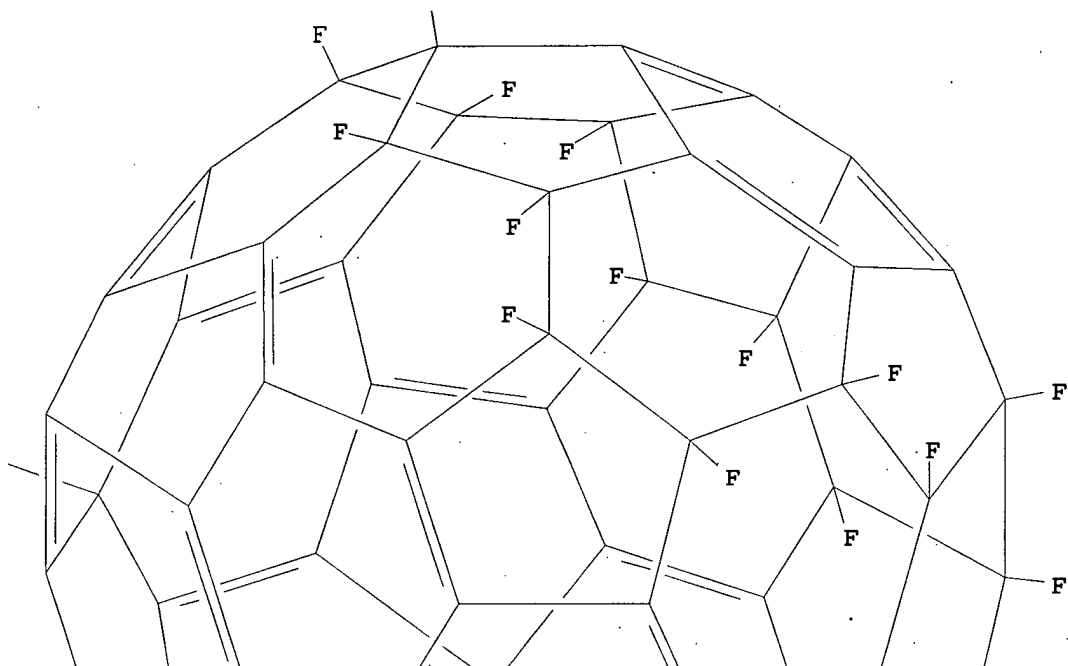
PAGE 1-B

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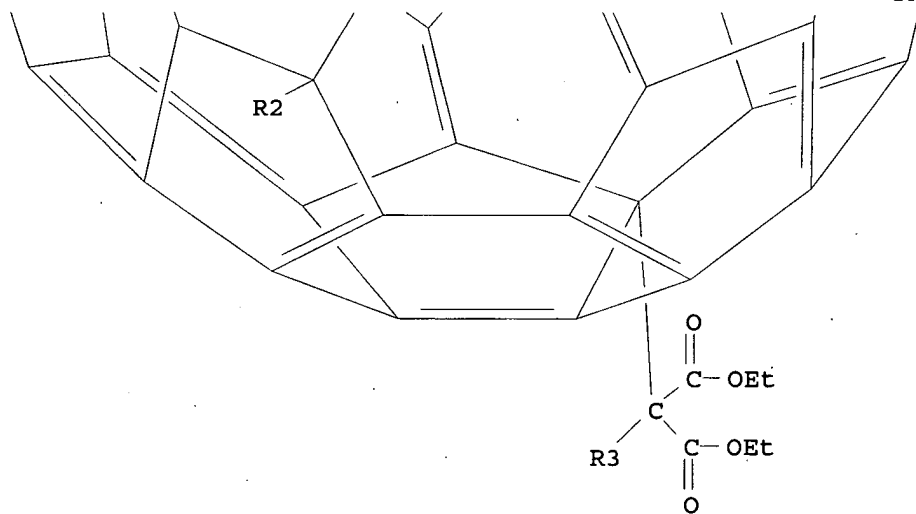
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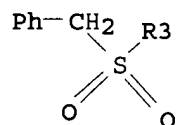
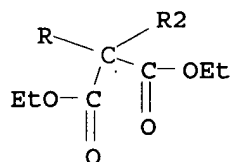
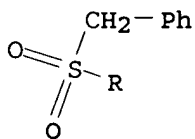
PAGE 2-B



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PAGE 4-A

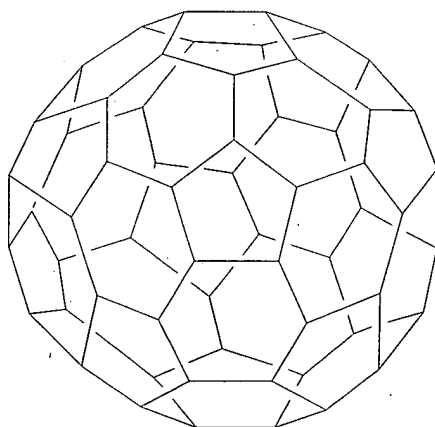


RN 591741-82-1 HCAPLUS  
 CN [5,6]Fullerene-C60-1h-diacetic acid,  $\alpha,\alpha'$ -dicyano-  
 $\alpha,\alpha'$ -bis(ethoxycarbonyl)hexadecafluorohexadecahydro-,  
 diethyl ester (9CI) (CA INDEX NAME)

CM 1

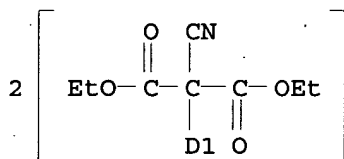
CRN 591741-81-0  
 CMF C76 H62 F16 N2 O8  
 CCI IDS

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16 ( D1-F )

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CC 22-4 (Physical Organic Chemistry)

IT 591722-01-9 591722-02-0

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(UV-Vis-NIR spectrum; steric effect on synthesis of 18 $\pi$  annulenic fluorofullerenes by nucleophilic substitution reaction of tertiary carbanions with C60F18)

IT 539825-96-2P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(electrochem. and conformational isomerism; steric effect on synthesis of 18 $\pi$  annulenic fluorofullerenes by nucleophilic substitution reaction of tertiary carbanions with C60F18)

IT 591721-96-9P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(electrochem.; steric effect on synthesis of 18 $\pi$  annulenic fluorofullerenes by nucleophilic substitution reaction of tertiary carbanions with C60F18)

IT 374623-61-7 475975-88-3

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent) (electronic absorption and reduction potential; steric effect on synthesis of 18 $\pi$  annulenic fluorofullerenes by nucleophilic substitution reaction of tertiary carbanions with C60F18)

IT 591721-95-8P 591721-97-0P 591721-98-1P

591741-80-9P 591741-82-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (steric effect on synthesis of 18 $\pi$  annulenic fluorofullerenes by nucleophilic substitution reaction of tertiary carbanions with C60F18)

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 17 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:363799 HCAPLUS

DOCUMENT NUMBER: 139:164613

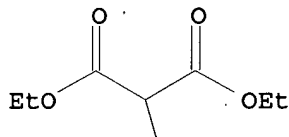
TITLE: Novel solvent-free reaction of C60 with active methylene compounds in the presence of Na2CO3 under high-speed vibration milling

AUTHOR(S): Wang, Guan-Wu; Zhang, Ting-Hu; Li, Yu-Jin; Lu, Ping; Zhan, Huan; Liu, You-Cheng; Murata, Yasujiro; Komatsu, Koichi

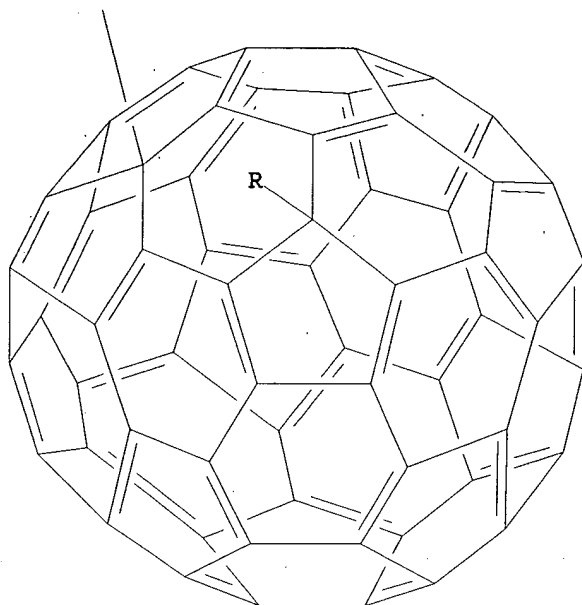
CORPORATE SOURCE: Department of Chemistry, University of Science and Technology of China, Hefei, Anhui, 230026,

SOURCE: Peop. Rep. China  
Tetrahedron Letters (2003), 44(23), 4407-4409  
CODEN: TELEAY; ISSN: 0040-4039  
PUBLISHER: Elsevier Science Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 139:164613  
AB Inorg. base, Na<sub>2</sub>CO<sub>3</sub>, was used to replace organic base, DBU, in the Bingel reaction employing di-Et bromomalonate under the mechanochem. high-speed vibration milling conditions to give the cyclopropanated C<sub>60</sub> in high yield. In contrast, reactions of C<sub>60</sub> with di-Et malonate and Et acetoacetate in the presence of Na<sub>2</sub>CO<sub>3</sub> under HSVM conditions afforded 1,4-bisadduct and dihydrofuran-fused C<sub>60</sub> derivative, resp.  
IT 573951-18-5P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(Bingel reaction of C<sub>60</sub> fullerene with di-Et bromomalonate using inorg. sodium carbonate base in place of organic base under vibration milling conditions to give 1,4-bisadduct)  
RN 573951-18-5 HCAPLUS  
CN [5,6]Fullerene-C<sub>60</sub>-1h-1,7-diacetic acid,  $\alpha,\alpha'$ -bis(ethoxycarbonyl)-, diethyl ester (9CI) (CA INDEX NAME)

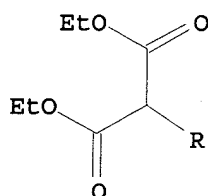
PAGE 1-A



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CC 25-29 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 Section cross-reference(s): 27

IT 573951-18-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (Bingel reaction of C60 fullerene with di-Et bromomalonate using  
 inorg. sodium carbonate base in place of organic base under  
 vibration milling conditions to give 1,4-bisadduct)

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE  
 FOR THIS RECORD. ALL CITATIONS AVAILABLE  
 IN THE RE FORMAT

L12 ANSWER 18 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:22293 HCAPLUS

DOCUMENT NUMBER: 139:28521

TITLE: A light-harvesting fluorinated fullerene  
 donor-acceptor ensemble; long-lived charge  
 separation

AUTHOR(S): Burley, Glenn A.; Avent, Anthony G.; Boltalina,  
 Olga V.; Gol'dt, Ilya V.; Guldi, Dirk M.;  
 Marcaccio, Massimo; Paolucci, Francesco;  
 Paolucci, Demis; Taylor, Roger

CORPORATE SOURCE: School of Chemistry, Physics and Environmental

Sciences, University of Sussex, Brighton, BN1 9QJ, UK

SOURCE: Chemical Communications (Cambridge, United Kingdom) (2003), (1), 148-149  
CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

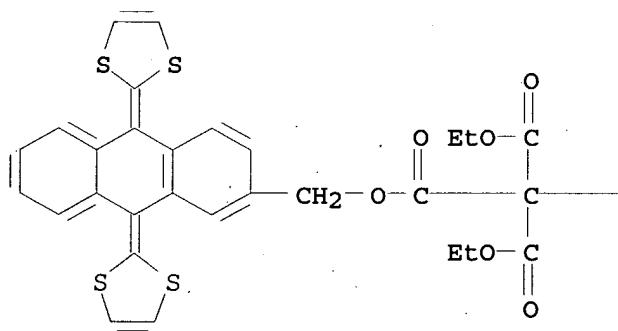
AB . Formation and photophys. properties are described of a novel multicomponent donor-acceptor dyad based on an all-trans 18 $\pi$  annulenic fluorofullerene (tranulene) with extended tetrathiafulvalene moieties. Visible light photoexcitation of tranulene-based dyad generated long-lived (870 ns) charge-separated state via rapid intramol. electron transfer. Electronic supplementary information (ESI) containing fluorescence spectra of the dyad and its Et ester (reference compound) and UV-visible spectra of the synthesized compds. is available at <http://www.rsc.org/suppdata/cc/b2/b209724a/>.

IT 539825-95-1P  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)  
(photoinduced intramol. electron transfer of donor-acceptor dyad based on annulenic fluorofullerene with extended tetrathiafulvalene moieties)

RN 539825-95-1 HCAPLUS

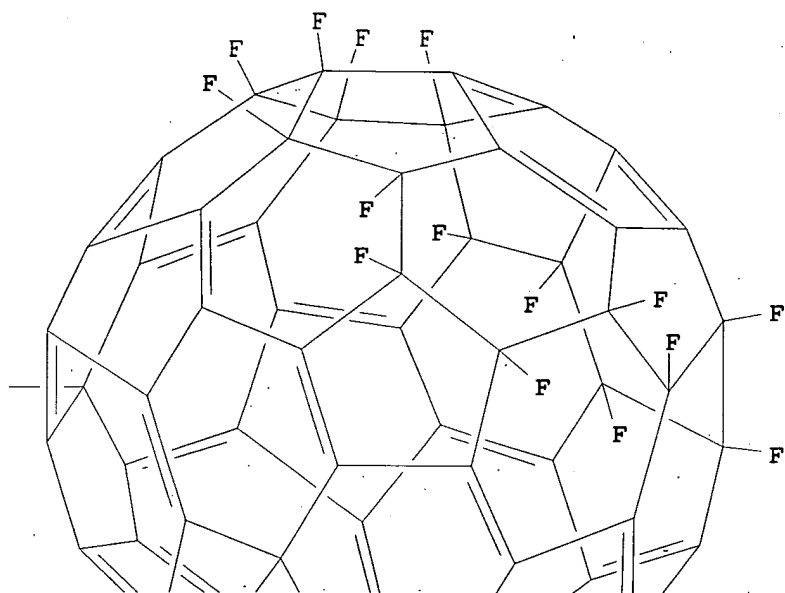
CN [5,6]Fullerene-C60-Ih-1,33,38(23H)-triacetic acid,  $\alpha,\alpha,\alpha',\alpha',\alpha'',\alpha''$ -hexakis(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-tetradecahydro-, tris[[9,10-bis(1,3-dithiol-2-ylidene)-9,10-dihydro-2-anthracenyl]methyl] ester (9CI) (CA INDEX NAME)

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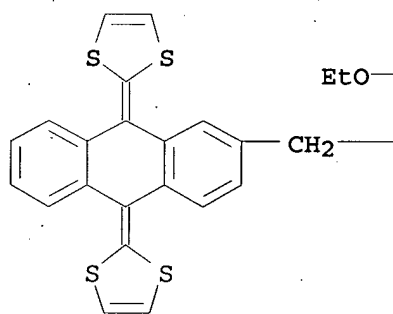




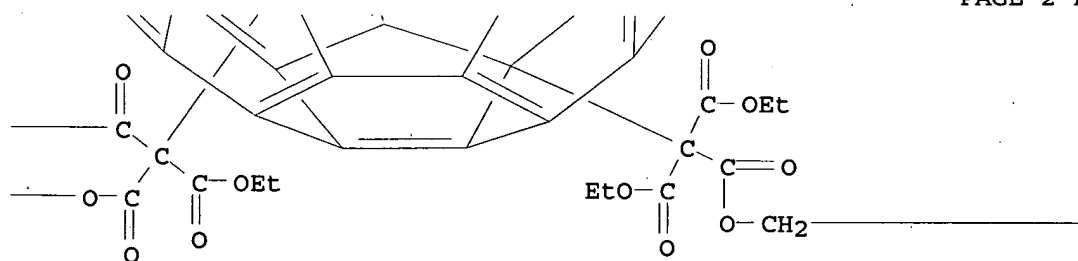
PAGE 1-B



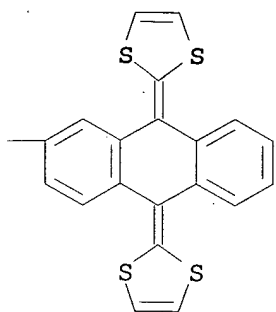
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IT 539825-96-2P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(reference compound; photoinduced intramol. electron transfer of donor-acceptor dyad based on annulenic fluorofullerene with extended tetrathiafulvalene moieties)

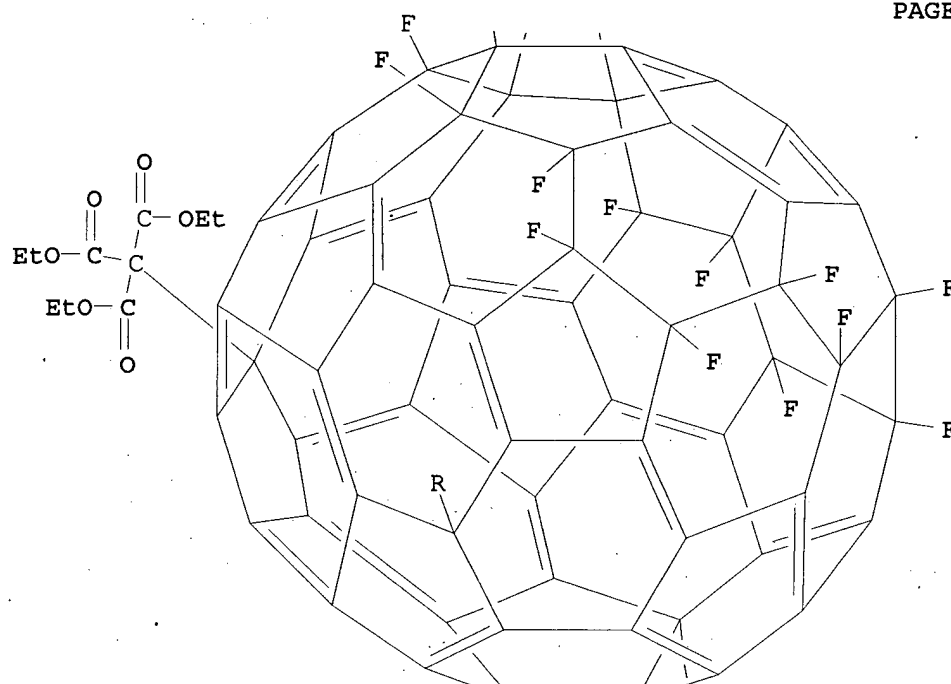
RN 539825-96-2 HCAPLUS

CN [5,6]Fullerene-C60-1h-1,33,38(23H)-triacetic acid,  $\alpha, \alpha, \alpha', \alpha', \alpha'', \alpha''$ -hexakis(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-tetradecahydro-, triethyl ester (9CI) (CA INDEX NAME)

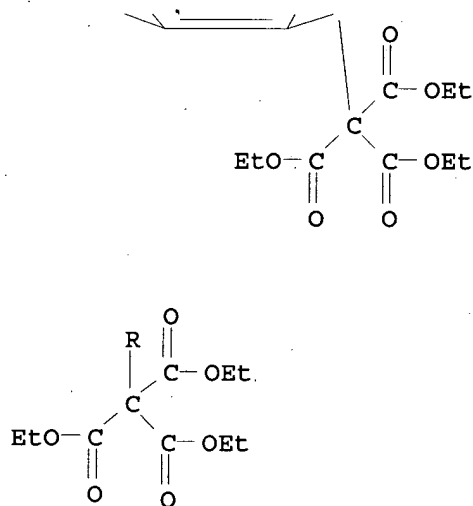
PAGE 1-A

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PAGE 2-A



PAGE 3-A



CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

IT 539825-95-1P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(photoinduced intramol. electron transfer of donor-acceptor dyad based on annulenic fluorofullerene with extended tetrathiafulvalene moieties)

IT 539825-96-2P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(reference compound; photoinduced intramol. electron transfer of donor-acceptor dyad based on annulenic fluorofullerene with extended tetrathiafulvalene moieties)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 19 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:977467 HCAPLUS

DOCUMENT NUMBER: 138:204967

TITLE: Synthesis and Properties of Bingel-type Methanofullerene- $\pi$ -Extended-TTF Diads and Triads

AUTHOR(S): Gonzalez, Susana; Martin, Nazario; Guldi, Dirk M.

CORPORATE SOURCE: Departamento de Quimica Organica, Facultad de Ciencias Quimicas, Universidad Complutense, Madrid, E-28040, Spain

SOURCE: Journal of Organic Chemistry (2003), 68(3), 779-791

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:204967

AB Novel C<sub>60</sub>/ $\pi$ -extended tetrathiafulvalene (exTTF) diads and triads [D2A (I) and DA2 (II)] have been synthesized by the Bingel cyclopropanation reaction of the resp. exTTF-containing malonates and [60]fullerene. The reaction of exTTF-bismalonates with C<sub>60</sub> affords the C<sub>60</sub>-exTTF diads (III) together with the triad C<sub>60</sub>-exTTF-C<sub>60</sub> (IV) and a regioisomeric mixture of bisadducts (V). Theor. calcns. (PM3) predict the favored geometry for triads I depending upon the orientation (up and down) of the 1,3-dithiole rings in the exTTFs, as well as the more stable regioisomers for the bisadducts V. Cyclic voltammetry measurements reveal that C<sub>60</sub> and exTTF units do not interact in the ground state. III and IV are not electrochem. stable. A photoinduced electron transfer leading to the formation of the radical pair (C<sub>60</sub>--exTTF<sup>•+</sup>) has been observed for compds. I.

IT 500004-11-5P 500004-12-6P 500004-13-7P

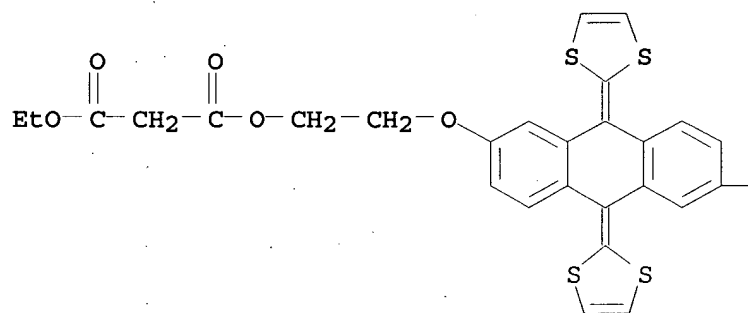
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(preparation and properties of Bingel-type methanofullerene- $\pi$ -extended-TTF diads and triads)

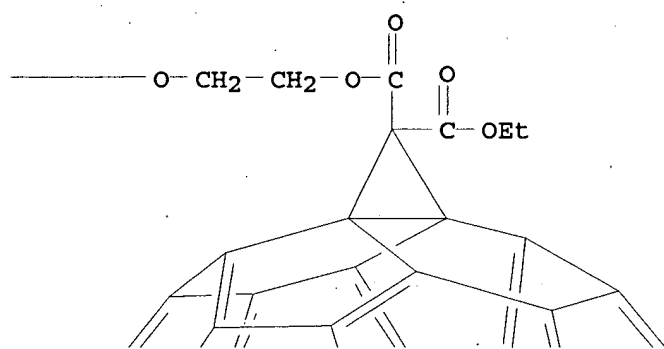
RN 500004-11-5 HCAPLUS

CN 3'H-Cyclopropa[1,9][5,6]fullerene-C<sub>60</sub>-Ih-3',3'-dicarboxylic acid, 2-[[9,10-bis(1,3-dithiol-2-ylidene)-6-[2-(3-ethoxy-1,3-dioxopropoxy)ethoxy]-9,10-dihydro-2-anthracenyl]oxy]ethyl ethyl ester (9CI) (CA INDEX NAME)

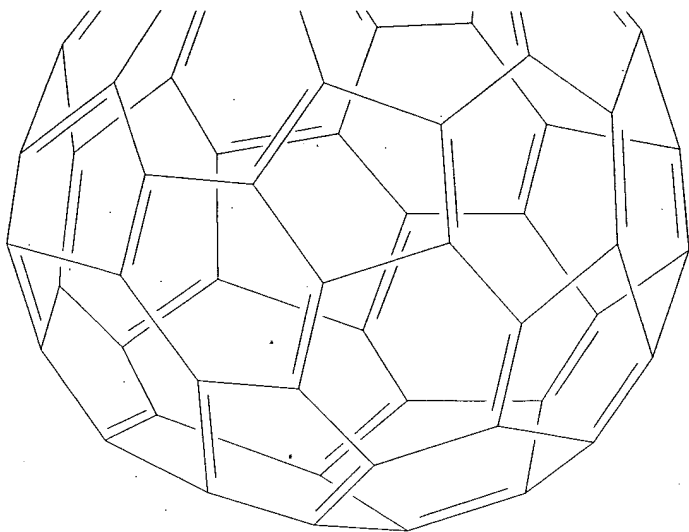
PAGE 1-A



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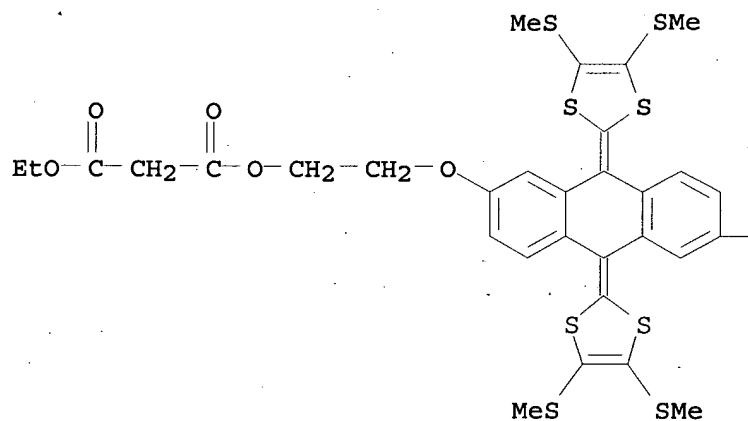


PAGE 2-B

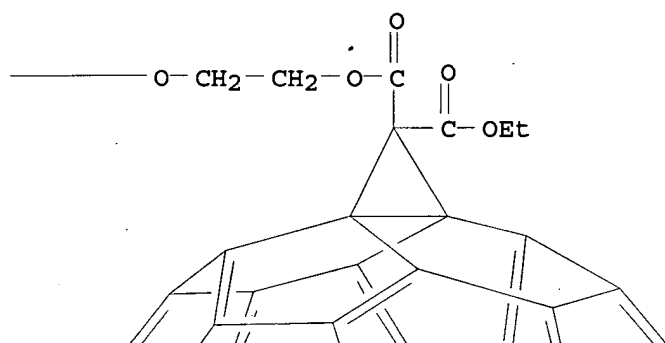


RN	500004-12-6	HCAPLUS
CN	3'H-Cyclopropa[1,9][5,6]fullerene-C60-1h-3',3'-dicarboxylic acid, 2-[[9,10-bis[4,5-bis(methylthio)-1,3-dithiol-2-ylidene]-6-[2-(3-ethoxy-1,3-dioxopropoxy)ethoxy]-9,10-dihydro-2-anthracenyl]oxy]ethyl ethyl ester (9CI) (CA INDEX NAME)	

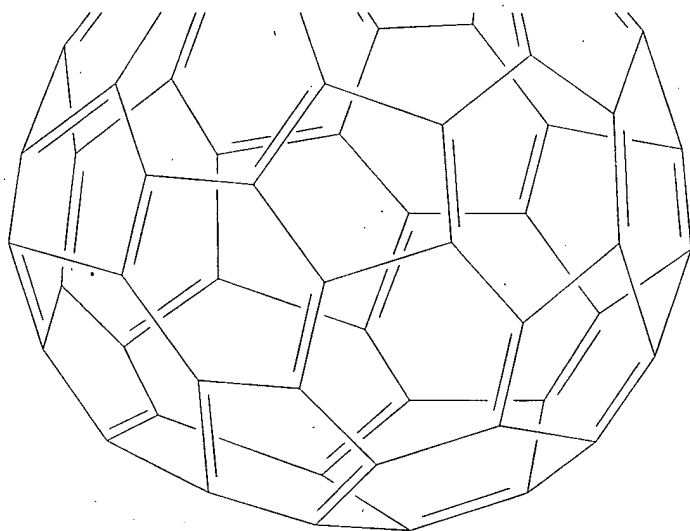
PAGE 1-A



PAGE 1-B

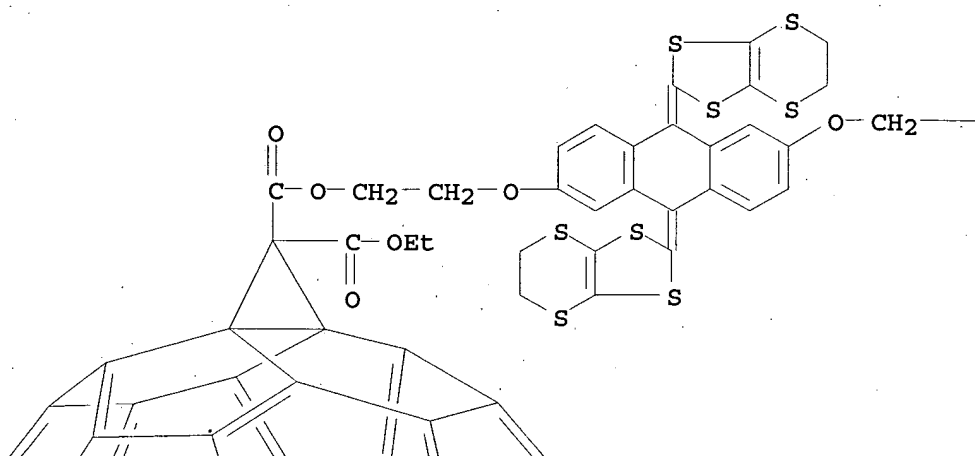


PAGE 2-B

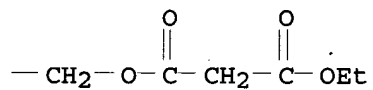


RN 500004-13-7 HCAPLUS  
 CN 3'H-Cyclopropa[1,9][5,6]fullerene-C60-1h-3',3'-dicarboxylic acid,  
 2-[[9,10-bis(5,6-dihydro-1,3-dithiolo[4,5-b][1,4]dithiin-2-ylidene)-  
 6-[2-(3-ethoxy-1,3-dioxopropoxy)ethoxy]-9,10-dihydro-2-  
 anthracenyl]oxy]ethyl ethyl ester (9CI) (CA INDEX NAME)

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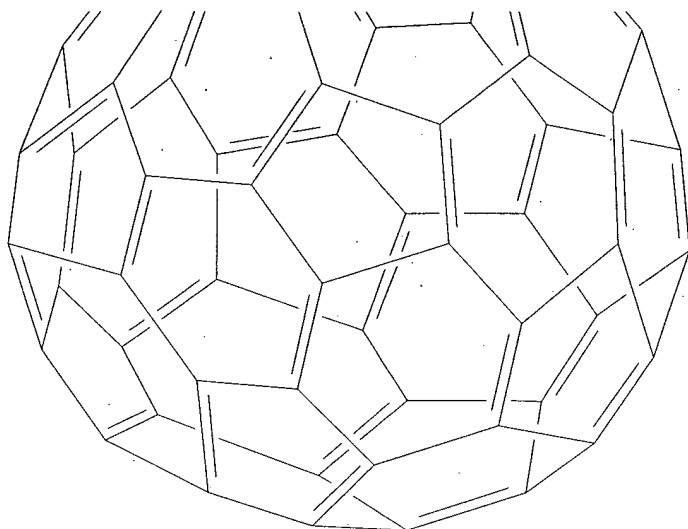


PAGE 1-B





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CC 28-5 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 73  
IT 99685-96-8DP, Fullerene C60, reaction products with  
bis-functionalized  $\pi$ -extended tetrathiafulvalenes 500003-91-8P  
500003-92-9P 500003-93-0P 500003-98-5P 500003-99-6P  
500004-00-2P 500004-07-9DP, bis-addition products with fullerene-C60  
500004-08-0DP, bis-addition products with fullerene-C60  
500004-09-1DP, bis-addition products with fullerene-C60 500004-10-4P  
500004-11-5P 500004-12-6P 500004-13-7P  
500004-14-8P 500004-15-9P 500004-16-0P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP  
(Preparation)

(preparation and properties of Bingel-type methanofullerene- $\pi$ -  
extended-TTF diads and triads)

REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE  
FOR THIS RECORD. ALL CITATIONS AVAILABLE  
IN THE RE FORMAT

L12 ANSWER 20 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:390961 HCAPLUS

DOCUMENT NUMBER: 137:384639

TITLE: Formation of [18]trannulenes derived via Bingel  
reactions between C60F18O isomers and  
CHBr(CO2Et)2 and between C60F18 and CHX(CO2R)2  
(X = Br, Cl; R = Me, Et)

AUTHOR(S): Darwish, Adam D.; Kuvytchko, Igor V.; Wei,  
Xian-Wen; Boltalina, Olga V.; Gol'dt, Ilya V.;  
Street, Joan M.; Taylor, Roger

CORPORATE SOURCE: The Chemistry Laboratory, CPES School,  
University of Sussex, Brighton, BN1 9QJ, UK

SOURCE: Journal of the Chemical Society, Perkin  
Transactions 2 (2002), (6), 1118-1121  
CODEN: JCSPGI; ISSN: 1472-779X

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:384639

AB Through extended  $\text{SN}_2'$  nucleophilic substitution of three fluorine atoms in two isomers of  $\text{C}_{60}\text{F}_{180}$  by alkyl halomalonate anions  $-\text{CBr}(\text{CO}_2\text{Et})_2$  (obtained from di-Et bromomalonate in the presence of DBU), we have prepared and characterized [18]trannulenes,  $\text{C}_{60}\text{F}_{150}[\text{CBr}(\text{CO}_2\text{Et})_2]_3$ . Likewise we have prepared [18]trannulenes by reactions between  $\text{C}_{60}\text{F}_{18}$  and either  $-\text{CBr}(\text{CO}_2\text{Me})_2$  or  $-\text{CCl}(\text{CO}_2\text{Et})_2$  (obtained from the corresponding esters and DBU). Formation of the trannulenes shows that the  $\text{CBr}(\text{CO}_2\text{Me})_2$  and  $\text{CCl}(\text{CO}_2\text{Et})_2$  substituents, though smaller than  $\text{CBr}(\text{CO}_2\text{Et})_2$ , are still large enough to bring about extended  $\text{SN}_2'$  substitution, rather than direct nucleophilic substitution. The products from the oxides show that oxygen does not inhibit trannulene formation either sterically or electronically. Each derivative has the brilliant emerald-green color of the corresponding [18]trannulene prepared from  $\text{C}_{60}\text{F}_{18}$  and di-Et bromomalonate, arising from bands at ca. 615 and 660 nm; minor variations in wavenumber and relative intensities occur according to the derivative. Under less forcing conditions, mono- and bis-substitution products were obtained from the more available sym. oxide and from reaction of the chloro and bromo esters with  $\text{C}_{60}\text{F}_{18}$ .

IT 475975-86-1P 475975-88-3P

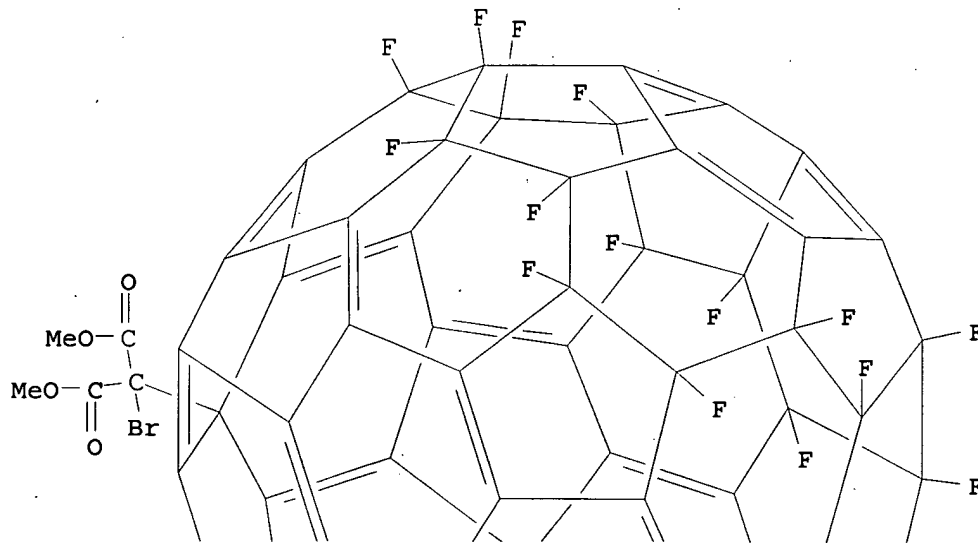
RL: SPN (Synthetic preparation); PREP (Preparation)

([18]trannulenes via Bingel reactions of  $\text{C}_{60}\text{F}_{180}$  isomers with di-Et bromomalonate)

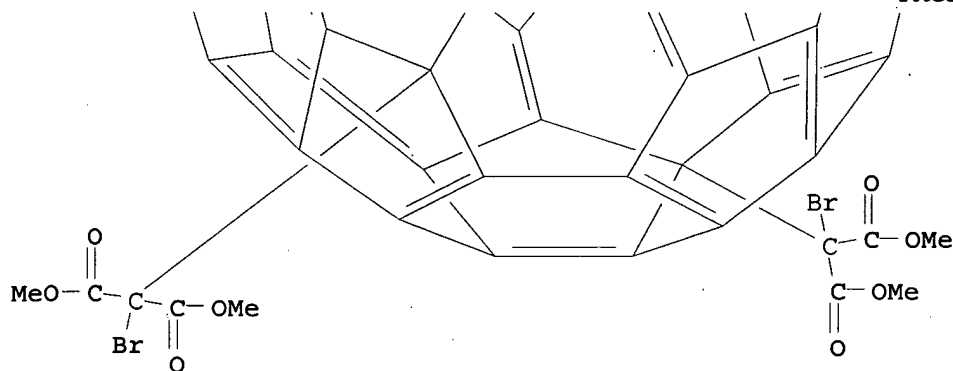
RN 475975-86-1 HCAPLUS

CN [5,6]Fullerene- $\text{C}_{60}$ -1h-1,33,38(23H)-triacetic acid,  $\alpha, \alpha', \alpha''$ -tribromo-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-tetradecahydro- $\alpha, \alpha', \alpha''$ -tris(methoxycarbonyl)-, trimethyl ester (9CI) (CA INDEX NAME)

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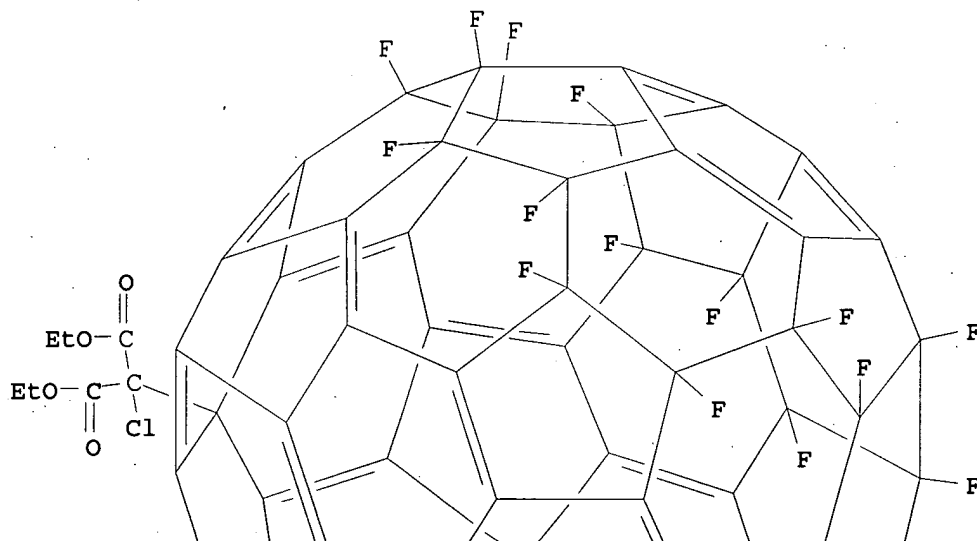


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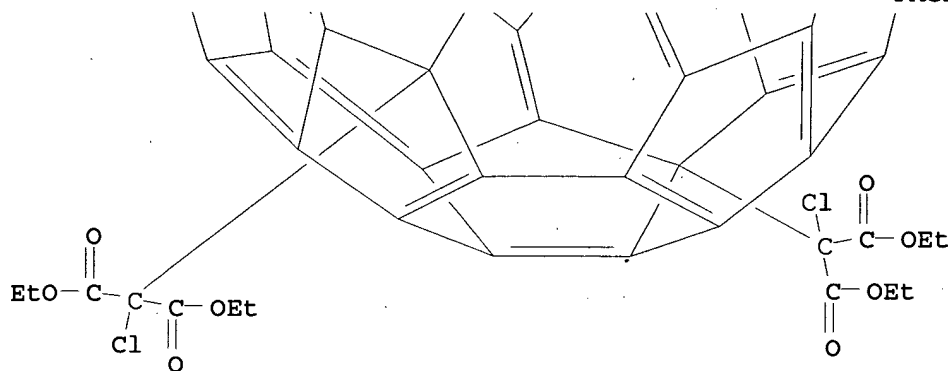


RN 475975-88-3 HCAPLUS  
 CN [5,6]Fullerene-C<sub>60</sub>-1h-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha',\alpha''$ -trichloro- $\alpha,\alpha',\alpha''$ -  
 tris(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
 tetradecafluoro-, triethyl ester (9CI) (CA INDEX NAME)

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CC 25-29 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 IT 475975-85-0P 475975-86-1P 475975-87-2P  
 475975-88-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 ([18]trannulenes via Bingel reactions of C60F18O isomers with  
 di-Et bromomalonate)

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE  
 FOR THIS RECORD. ALL CITATIONS AVAILABLE  
 IN THE RE FORMAT

L12 ANSWER 21 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:196621 HCAPLUS

DOCUMENT NUMBER: 137:6171

TITLE: Th-symmetrical hexakisadducts of C60 with a  
 densely packed  $\pi$ -donor shell can act as  
 energy- or electron-transducing systems

AUTHOR(S): Diekers, Michael; Luo, Chuping; Guldi, Dirk M.;  
 Hirsch, Andreas

CORPORATE SOURCE: Institut fur Organische Chemie Universitat  
 Erlangen-Nurnberg, Erlangen, 91054, Germany

SOURCE: Chemistry--A European Journal (2002), 8(4),  
 979-991

CODEN: CEUJED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:6171

AB For the first time several Th-sym. hexakisadducts of C60 bearing up  
 to six electro- and photoactive o-phenylene diamine or  
 9,10-dialkoxyanthracene moieties were synthesized and subjected to  
 photoinduced electron/energy-transfer studies. Both donors form a  
 densely packed  $\pi$ -donor shell surrounding the fullerene core. In  
 these novel core-shell ensembles either an efficient energy transfer  
 from the dialkoxyanthracene periphery, or an electron transfer from  
 the o-phenylene diamine periphery transducers the flow of  
 excited-state energy or electrons, resp., to the fullerene moiety,  
 which resides in the central core. Due to the relatively high reduction  
 potential of the fullerene core, which is anodically shifted by  
 $\approx 0.7$  V, compared with that of pristine C60, the outcome of  
 these intramol. reactions depends mainly on the donor ability of the  
 peripheral system. Interestingly, the charge-separated state in the  
 o-phenylene diamine heptad ( $\tau = 2380$  ns in benzonitrile) is  
 stabilized by a factor of 20 relative to the corresponding

o-phenylene diamine dyad ( $\tau = 120$  ns in benzonitrile), an effect that points unequivocally to the optimized storage of charges in this highly functionalized fullerene ensemble.

IT 433718-12-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of Th-sym. fullerene-C60 hexakisadducts with densely packed  $\pi$ -donor shell and their properties as energy- or electron-transducing systems)

RN 433718-12-8 HCAPLUS

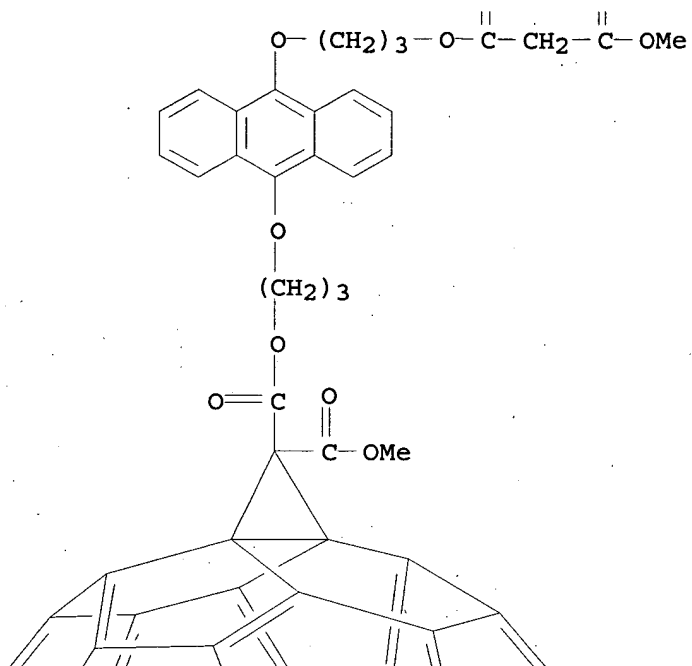
CN 3'H-Cyclopropa[1,9][5,6]fullerene-C60-Ih-3',3'-dicarboxylic acid,  
3-[[10-[3-(3-methoxy-1,3-dioxopropoxy)propoxy]-9-anthracenyl]oxy]propyl methyl ester (9CI) (CA INDEX NAME)

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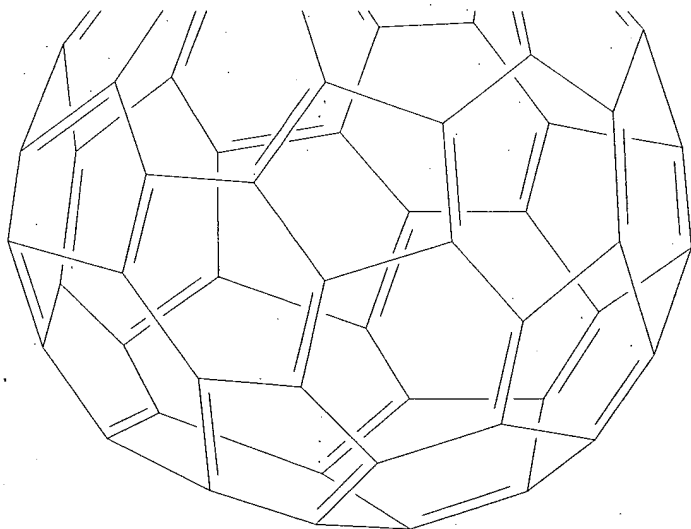
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CC 28-23 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 22

IT 433718-12-8P 433718-13-9P 433718-14-0P 433718-15-1P  
 433718-16-2P 433718-18-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of Th-sym. fullerene-C60 hexakisadducts with densely packed  $\pi$ -donor shell and their properties as energy- or

electron-transducing systems)

REFERENCE COUNT: 63 THERE ARE 63 CITED REFERENCES AVAILABLE  
FOR THIS RECORD. ALL CITATIONS AVAILABLE  
IN THE RE FORMAT

L12 ANSWER 22 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:71160 HCAPLUS

DOCUMENT NUMBER: 136:278984

TITLE: Reaction of C60F18 with diethyl bromomalonate:  
diversion of the Bingel reaction and formation  
of the first 18 $\pi$  annulenic fullerene

AUTHOR(S): Wei, Xian-Wen; Avent, Anthony G.; Boltalina,  
Olga V.; Darwish, Adam D.; Fowler, Patrick W.;  
Sandall, John P. B.; Street, Joan M.; Taylor,  
Roger

CORPORATE SOURCE: The Chemistry Laboratory, CPES School, Sussex  
University, Brighton, BN1 9QJ, UK

SOURCE: Journal of the Chemical Society, Perkin  
Transactions 2 (2002), (1), 41-46  
CODEN: JCSPGI; ISSN: 1472-779X

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:278984

AB Reaction of C60F18 with di-Et bromomalonate in the presence of DBU results in the nucleophilic replacement of either one, two, or three of the most accessible fluorine atoms by CBr(CO2Et)2 moieties, in preference to formation of a cyclopropanated derivative (the normal Bingel reaction). Substitution that takes place  $\delta$  to the departing fluorine, is the first proven example of SN2' substitution in a fullerene, and appears to be sterically driven. The ratio of mono-/poly-substitution products can be controlled by varying the rate of addition of the DBU and the molar ratio between C60F18 and the other reagents. The tri-substituted product is an [18]annulene, has an intense emerald-green color ascribable to the electron delocalization in the (equatorial) annulene belt (bond length variation 0.018 Å), and has C3v symmetry. This is the first example on an annulenic fullerene (moreover of an all-trans annulene or trannulene). The extent of substitution in each compound is identified from the fluorinated fragments (C60F15, C60F16, and C60F17, resp., for tri-, di-, and mono-substitution) in the EI mass spectra, and by their 1H and 19F NMR spectra. The structure of the tri-substituted [18]annulene was confirmed by single crystal X-ray diffraction. Normal Bingel cycloaddn. also takes place between C60F18 and di-Et malonate-DBU in CBr4, to give C60F18C(CO2Et)2 and C60F16C(CO2Et)2 in relatively low yields. Calcns. indicate a critical size of substituent required to produce  $\delta$ -substitution, rather than ipso-substitution of the departing fluorine.

IT 374623-61-7P 405910-74-9P

RL: PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)

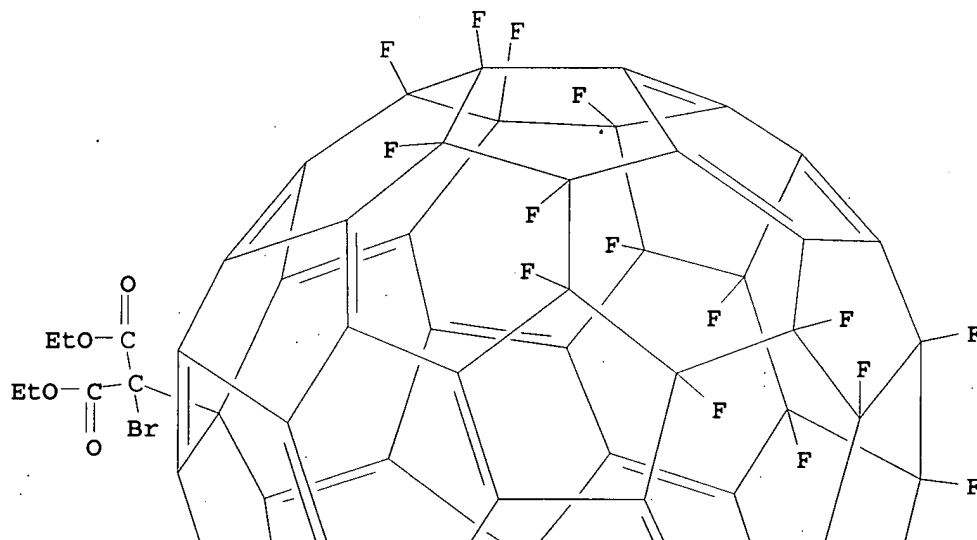
(nucleophilic substitution reaction of C60F18 with di-Et bromomalonate in preference to the Bingel reaction resulting in the formation of the first 18 $\pi$  annulenic fullerene (trannulene))

RN 374623-61-7 HCAPLUS

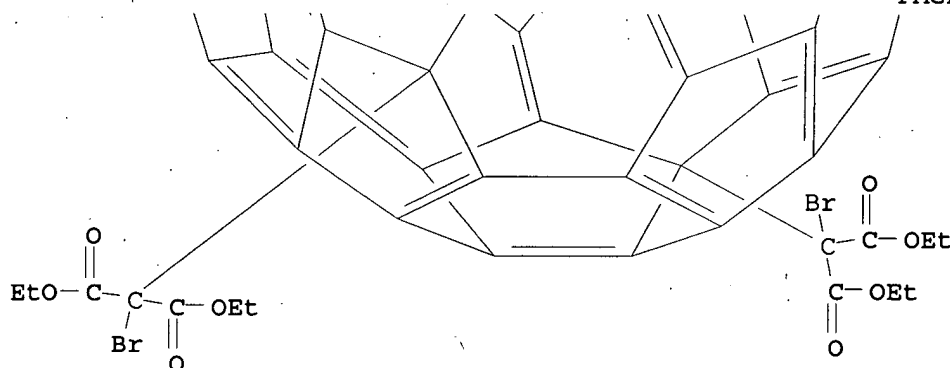
CN [5,6]Fullerene-C60-1h-1,33,38(23H)-triacetic acid,  
 $\alpha,\alpha',\alpha''$ -tribromo- $\alpha,\alpha',\alpha''$ -  
tris(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-  
pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-

tetradecahydro-, triethyl ester (9CI) (CA INDEX NAME)

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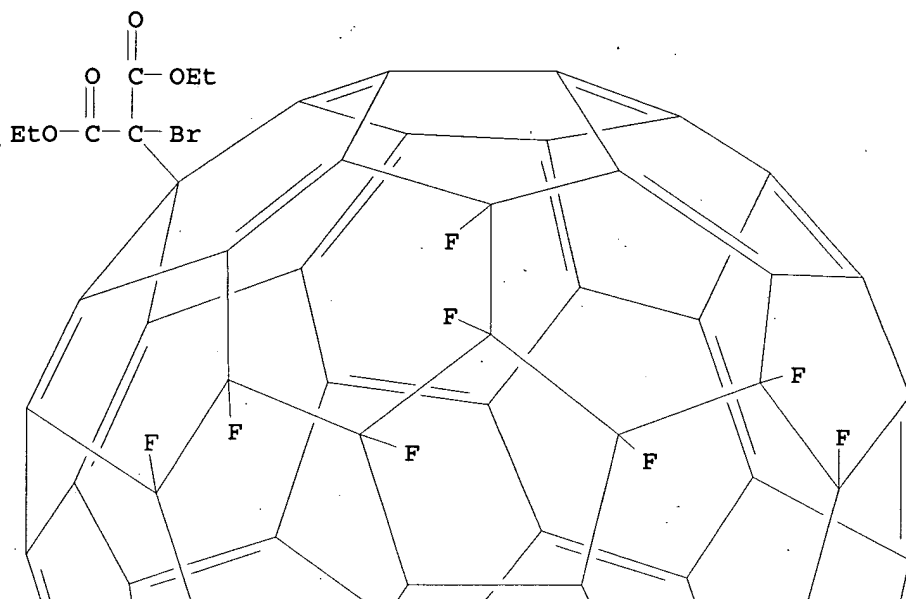
PAGE 2-A



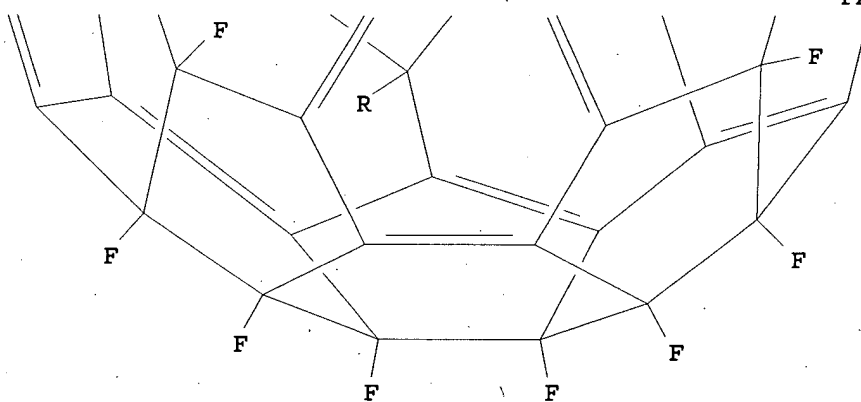
RN 405910-74-9 HCAPLUS  
 CN [5,6]Fullerene-C<sub>60</sub>-1h-1,33-diacetic acid,  $\alpha,\alpha'$ -dibromo-  
 $\alpha,\alpha'$ -bis(ethoxycarbonyl)-22,23,24,25,26,27,28,41,42,47,4  
 8,49,55,56,59,60-hexadecafluoro-22,23,24,25,26,27,28,41,42,47,48,49,  
 55,56,59,60-hexadecahydro-, diethyl ester (9CI) (CA INDEX NAME)



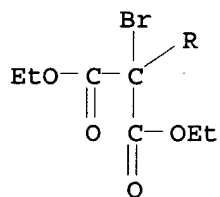
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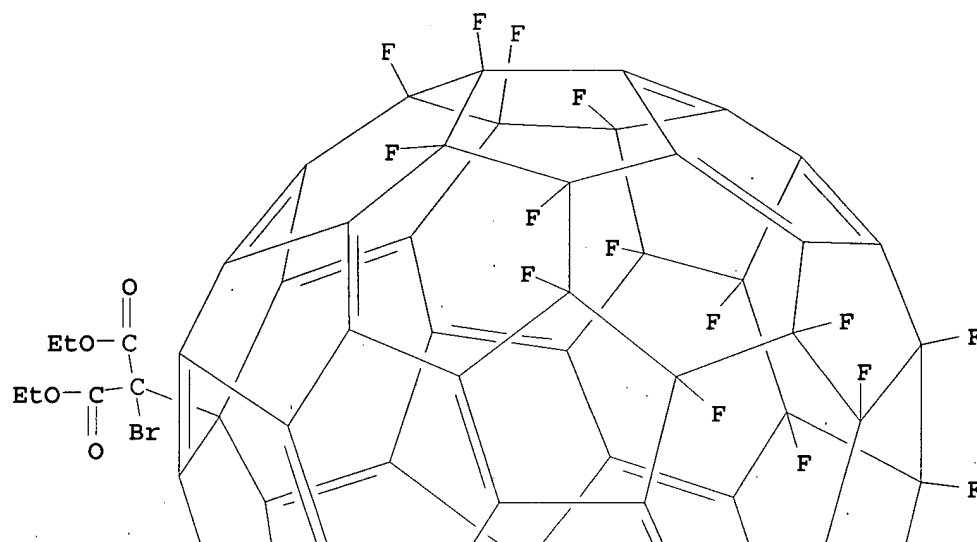


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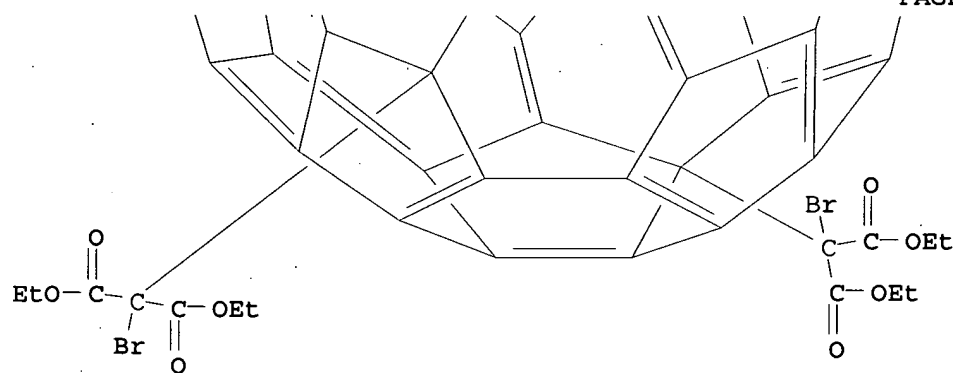


Section cross-reference(s): 75  
IT 90762-52-ODP, [18]Trannulene, embedded on fullerene surface  
374623-61-7P 405910-74-9P 405910-75-0P  
405910-76-1P 405917-50-2P  
RL: PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)  
(nucleophilic substitution reaction of C60F18 with di-Et bromomalonate in preference to the Bingel reaction resulting in the formation of the first 18 $\pi$  annulenic fullerene (trannulene))  
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT  
  
L12 ANSWER 23 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2001:665860 HCAPLUS  
DOCUMENT NUMBER: 135:371515  
TITLE: The remarkable stable emerald green C60F15[CBr(CO2Et)2]3: The first [60] fullerene that is also the first [18] trannulene  
AUTHOR(S): Wei, Xian-Wen; Darwish, Adam D.; Boltalina, Olga V.; Hitchcock, Peter B.; Street, Joan M.; Taylor, Roger  
CORPORATE SOURCE: School of Chemistry, Physics & Environmental Sciences, Sussex University, Brighton, BN1 9QJ, UK  
SOURCE: Angewandte Chemie, International Edition (2001), 40(16), 2989-2992  
CODEN: ACIEF5; ISSN: 1433-7851  
PUBLISHER: Wiley-VCH Verlag GmbH  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 135:371515  
AB The title compound was obtained by treating C60F18 with BrCH(CO2Et)2 and was characterized via its crystal structure and spectral data.  
IT 374623-62-8P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal and mol. structure of C60F15[CBr(CO2Et)2]3)  
RN 374623-62-8 HCAPLUS  
CN [5,6]Fullerene-C60-Ih-1,33,38(23H)-triacetic acid,  $\alpha,\alpha',\alpha''$ -tribromo- $\alpha,\alpha',\alpha''$ -tris(ethoxycarbonyl)-23,24,25,26,27,28,41,42,47,48,49,55,56,59,60-pentadecafluoro-24,25,26,27,28,41,42,47,48,49,55,56,59,60-tetradecahydro-, triethyl ester, compd. with methylbenzene (1:1) (9CI) (CA INDEX NAME)  
  
CM 1  
  
CRN 374623-61-7  
CMF C81 H30 Br3 F15 O12

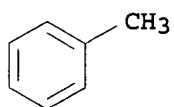
PAGE 1-A



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CM 2

CRN 108-88-3  
CMF C7 H8

CC 25-29 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
IT 374623-62-8P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP  
(Preparation)  
(preparation and crystal and mol. structure of C60F15[CBr(CO2Et)2]3)  
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE  
FOR THIS RECORD. ALL CITATIONS AVAILABLE  
IN THE RE FORMAT

L12 ANSWER 24 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:418173 HCAPLUS

DOCUMENT NUMBER: 135:226976

TITLE: Hexakis-adducts of [60]fullerene with different  
addition patterns: templated synthesis, physical  
properties, and chemical reactivity

AUTHOR(S): Bourgeois, Jean-Pascal; Woods, Craig R.;  
Cardullo, Francesca; Habicher, Tilo;  
Nierengarten, Jean-Francois; Gehrig, Regula;  
Diederich, Francois

CORPORATE SOURCE: Laboratorium fur Organische Chemie, ETH-Zentrum,  
Zurich, CH-8092, Switz.

SOURCE: Helvetica Chimica Acta (2001), 84(5), 1207-1226  
CODEN: HCACAV; ISSN: 0018-019X

PUBLISHER: Verlag Helvetica Chimica Acta

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:226976

AB Representatives of two classes of hexakis-adducts of C60 were prepared by templated synthesis strategies. Fullerene with a dipyridylmethano addend in a pseudo-octahedral addition pattern was obtained by 9,10-dimethylantracene-templated addition and served as the starting material for the first supramol. fullerene dimer. A hexakis-adduct, also possessing a pseudo-octahedral addition pattern, was obtained by a sequence of tether-directed remote functionalization, tether removal, and regioselective bis-functionalization. With its two diethynylmethano addends in trans-1 position, it is a precursor for fascinating new oligomers and polymers that feature C60 moieties as part of the polymeric backbone. With the residual fullerene  $\pi$ -electron chromophore reduced to a "cubic cyclophane"-type sub-structure and for steric reasons, these compds. no longer display electrophilic reactivity. As a representative of the second class of hexakis-adducts, an adduct which features six addends in a distinct helical array along an equatorial belt was prepared by a route that involved two sequential tether-directed remote functionalization steps. In this compound  $\pi$ -electron conjugation between the two unsubstituted poles of the carbon sphere is maintained via two (E)-stilbene-like bridges. As a result, this compound features very different chemical reactivity and phys. properties when compared to hexakis-adducts with a pseudo-octahedral addition pattern. Its reduction under cyclic voltammetric conditions is greatly facilitated (by 570 mV), and it readily undergoes addnl., electronically favored Bingel addns. at the two sterically well-accessible central polar 6-6 bonds under formation of heptakis- and octakis-adducts. The different extent of the residual  $\pi$ -electron delocalization in the fullerene sphere is also reflected in the optical properties of the two types of hexakis-adducts. Whereas the first two adducts are bright-yellow (end-absorption around 450 nm), the last-named compound is shiny-red, with an end-absorption around 600 nm. This study once more demonstrates the power of templated functionalization strategies in

fullerene chemical, providing addition patterns that are not accessible by stepwise synthetic approaches.

IT 321402-57-7P

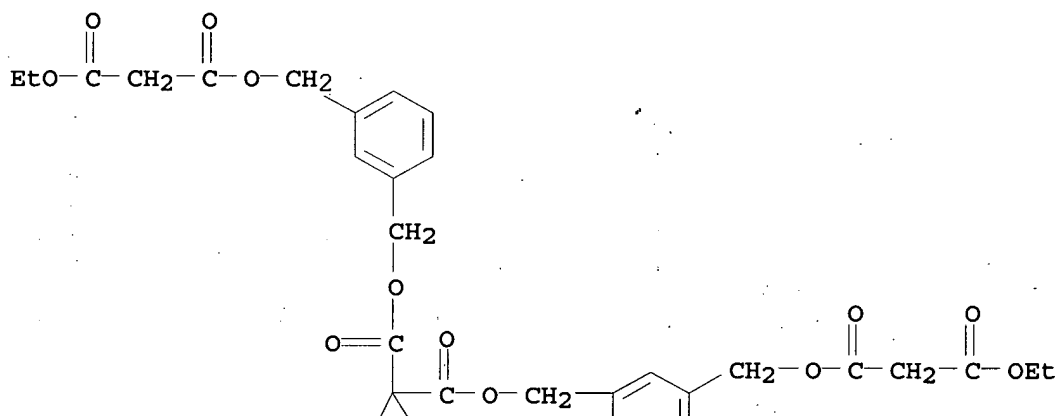
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
 RACT (Reactant or reagent)

(preparation, phys. properties, and chemical reactivity of  
 hexakis-adducts of [60]fullerene with different addition patterns)

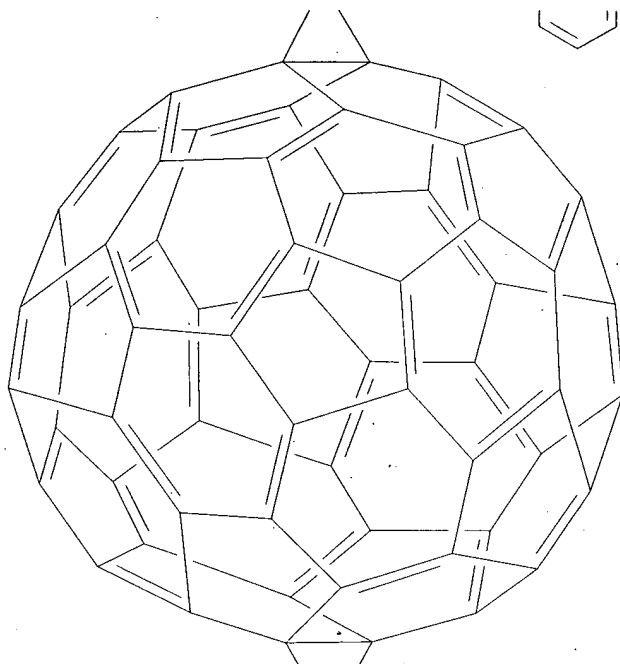
RN 321402-57-7 HCAPLUS

CN 3'H,3''H-Dicyclopropa[1,9:52,60][5,6]fullerene-C60-Ih-3',3'',3''',3''''-  
 tetracarboxylic acid, tetrakis[3-[(3-ethoxy-1,3-  
 dioxopropoxy)methyl]phenyl]methyl ester (9CI) (CA INDEX NAME)

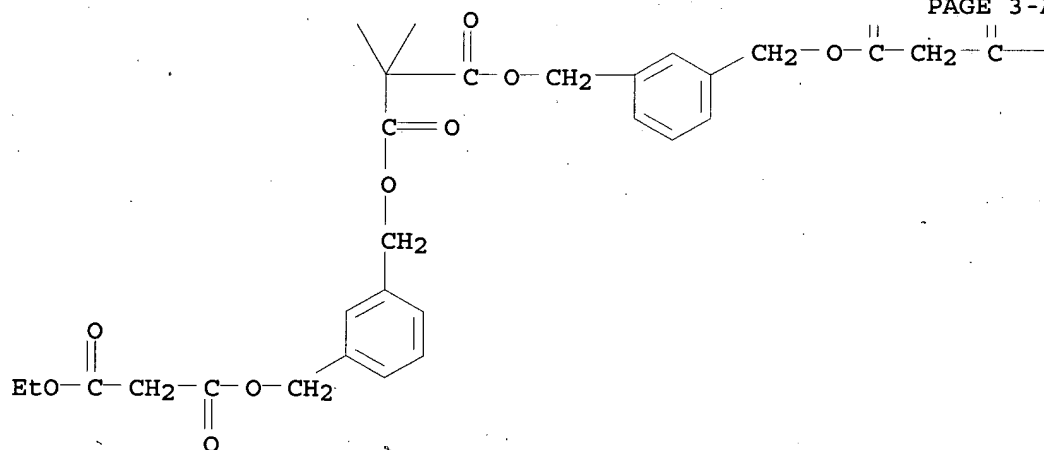
PAGE 1-A



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PAGE 3-B

—OEt

CC 28-23 (Heterocyclic Compounds (More Than One Hetero Atom))  
 IT 212846-70-3P 212846-78-1P 214076-93-4P 321402-51-1P  
 321402-53-3P 321402-55-5P 321402-57-7P 331812-40-9P  
 358376-63-3P 358376-64-4P 358376-66-6P 358376-67-7P

358376-68-8P 358376-71-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
RACT (Reactant or reagent)(preparation, phys. properties, and chemical reactivity of  
hexakis-adducts of [60]fullerene with different addition patterns)REFERENCE COUNT: 85 THERE ARE 85 CITED REFERENCES AVAILABLE  
FOR THIS RECORD. ALL CITATIONS AVAILABLE  
IN THE RE FORMAT

L12 ANSWER 25 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:88056 HCAPLUS

DOCUMENT NUMBER: 134:280592

TITLE: The chemical retro-Bingel reaction: selective  
removal of bis(alkoxycarbonyl)methano addends  
from C60 and C70 with amalgamated magnesiumAUTHOR(S): Thilgen, Carlo; Moonen, Nicolle N. P.; Schmitt,  
Jean-Louis; Kessinger, Roland; Diederich,  
FrancoisCORPORATE SOURCE: Laboratorium fur Organische Chemie, ETH-Zentrum,  
Zurich, CH-8092, Switz.SOURCE: Proceedings - Electrochemical Society (2000),  
2000-11(Fullerenes 2000--Volume 9:  
Functionalized Fullerenes), 85-91  
CODEN: PESODO; ISSN: 0161-6374

PUBLISHER: Electrochemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:280592

AB Bis(alkoxycarbonyl)methano addends can be removed from C60 and C70  
derivs. by reaction with amalgamated magnesium in refluxing THF.  
This facile and selective chemical retro-Bingel reaction does not  
affect pyrrolidine rings fused to C60, thus opening up the  
possibility of using Bingel type addends as temporary protecting and  
directing groups in the regioselective synthesis of multiple adducts  
with uncommon functionalization patterns.

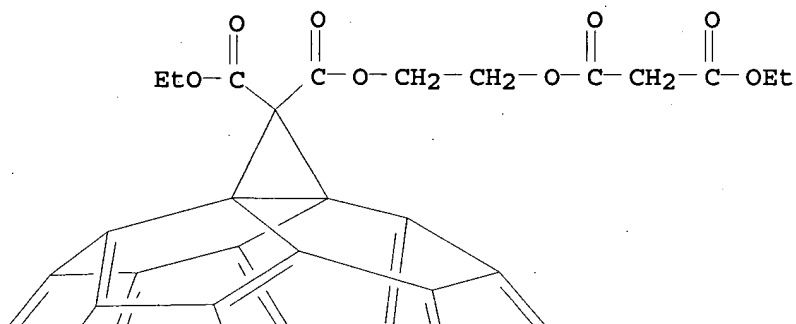
IT 293768-14-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(chemical retro-Bingel reaction of bis(alkoxycarbonyl)methano  
addends from C60 and C70)

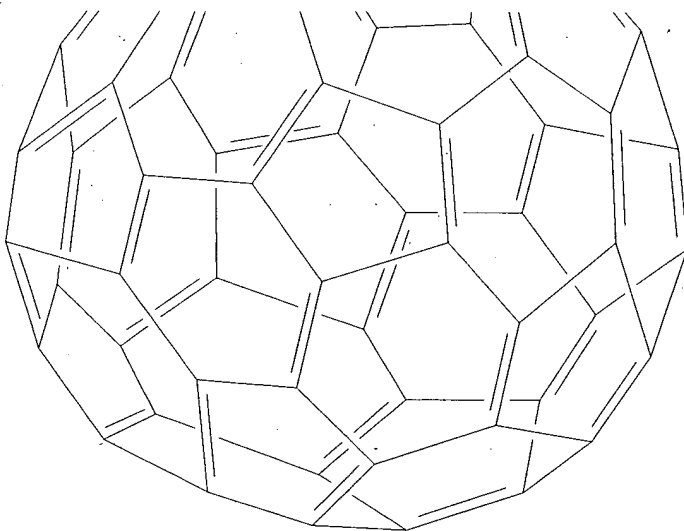
RN 293768-14-6 HCAPLUS

CN 3'H-Cyclopropa[1,9][5,6]fullerene-C60-1h-3',3'-dicarboxylic acid,  
2-(3-ethoxy-1,3-dioxopropoxy)ethyl ethyl ester (9CI) (CA INDEX  
NAME)

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CC 25-29 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

Section cross-reference(s): 27, 28

IT 99685-96-8P, C60 Fullerene 115383-22-7P, C70 Fullerene

151872-44-5P **293768-14-6P**

RL: SPN (Synthetic preparation); PREP (Preparation)

(chemical retro-Bingel reaction of bis(alkoxycarbonyl)methane addends from C60 and C70)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE  
FOR THIS RECORD. ALL CITATIONS AVAILABLE  
IN THE RE FORMAT

L12 ANSWER 26 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:48514 HCAPLUS

DOCUMENT NUMBER: 134:266287

TITLE: Optically active macrocyclic cis-3 bis-adducts  
of C60: regio- and stereoselective synthesis,  
exciton chirality coupling, and determination of  
the absolute configuration, and first  
observation of exciton coupling between  
fullerene chromophores in a chiral environment

AUTHOR(S): Kessinger, Roland; Thilgen, Carlo; Mordasini,  
Tiziana; Diederich, Francois

CORPORATE SOURCE: Laboratorium fur Organische Chemie, ETH-Zentrum,  
Zurich, CH-8092, Switz.

SOURCE: Helvetica Chimica Acta (2000), 83(12), 3069-3096  
CODEN: HCACAV; ISSN: 0018-019X

PUBLISHER: Verlag Helvetica Chimica Acta

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:266287

AB A series of optically active cis-3 bis-adducts was obtained regio- and diastereoselectively by Bingel macrocyclization of C60 with bis-malonates, which contain optically active tethers derived from 1,2-diols. The absolute configuration of the inherently chiral addition pattern in cis-3 bis-adducts had previously been determined by comparison of calculated and exptl. CD spectra. Full confirmation of these earlier assignments was now obtained by an independent method based on semiempirical AM1 and OM2 calcns. combined with 1H-NMR spectroscopy. It was found computationally that bis-malonates [RCH(O2CCH2CO2Et)]2, which contain (R,R)- or (S,S)-butane-2,3-diol derivs. as optically active tethers, preferentially form out-out cis-3 bis-adducts of C60 as a single diastereoisomer in which the alkyl groups R adopt a gauche conformation, while the two glycolic H-atoms are in an antiperiplanar (ap) and the ester linkages to the fullerene in a gauche relationship. In contrast, in the less favorable diastereoisomer, which should not form, the alkyl groups R adopt an ap and the H-atoms a gauche conformation, while the ester bridges to the fullerene remain, for geometric reasons, locked in a gauche conformation. According to the OM2 calcns., the geometry of the fully staggered tether in the free bis-malonates closely resembles the conformation of the tether fragment in the bis-adducts formed. These computational predictions were confirmed exptl. by the measurement of the coupling constant between the vicinal glycolic H-atoms in the 1H-NMR spectrum. This conformational anal. was further supported by the regio- and diastereoselective synthesis of cis-3 bis-adducts from bis-malonates, including tethers derived from cyclic glycol units with a fixed gauche conformation of the alkyl residues R at the glycolic C-atoms. Thus, a bis-malonate of (R,R)-cyclohexane-1,2-diol provided exclusively cis-3 bis-adduct. Incorporation of a tether derived from Me 4,6-O,O-benzylidene- $\alpha$ -D-glucopyranoside into the bis-malonate and Bingel macrocyclization diastereoselectively produced the cis-3 stereoisomer as the only macrocyclic bis-adduct. If the geometry of the alkyl groups R at the glycolic C-atoms of the tether component deviates from a gauche relationship, as in the case of tethers derived from exo cis- and trans-norbornane-2,3-diol or from trans-cyclopentane-1,2-diol, hardly any macrocyclic product is

formed. The absolute configurations of the various optically active cis-3 bis-adducts were also assigned by comparison of their CD spectra, which are dominated by the chiroptical contributions of the inherently chiral fullerene chromophore. A strong chiral exciton coupling was observed for optically active macrocyclic cis-3 bis-adducts of C<sub>60</sub> with two appended 4-(dimethylamino)benzoate or meso-tetraphenylporphyrin chromophores. Chiral exciton coupling between two fullerene chromophores was observed for the first time in the CD spectrum of the threitol-bridged bis-fullerene.

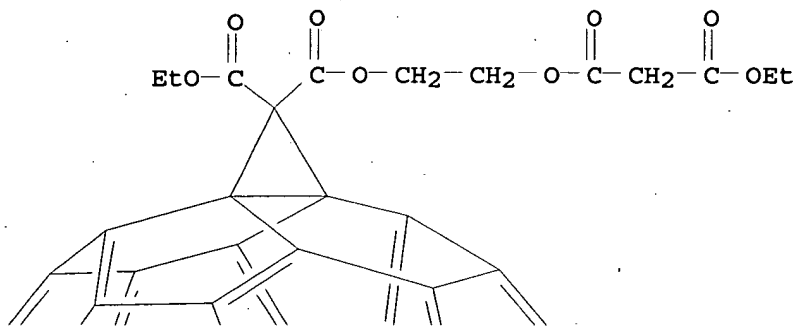
IT 293768-14-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation, conformation, and exciton coupling of macrocyclic adducts of fullerene with bismalonates)

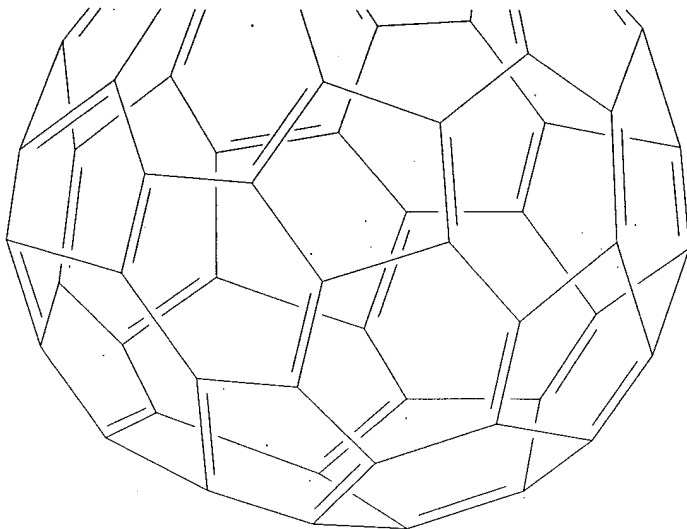
RN 293768-14-6 HCAPLUS

CN 3'H-Cyclopropa[1,9][5,6]fullerene-C60-1h-3',3'-dicarboxylic acid,  
2-(3-ethoxy-1,3-dioxopropoxy)ethyl ethyl ester (9CI) (CA INDEX  
NAME)

PAGE 1-A



PAGE 2-A



CC 28-23 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 22, 25

IT 293768-14-6P 331812-42-1P 331812-43-2P 331812-44-3P  
331812-48-7P 331812-49-8P 331812-51-2P 331812-53-4P  
331812-57-8P 331812-61-4P 331812-66-9P 331839-43-1P  
331839-44-2P 331839-46-4P 331839-47-5P 331839-49-7P  
331839-50-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation, conformation, and exciton coupling of macrocyclic  
adducts of fullerene with bismalonates)

REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE  
FOR THIS RECORD. ALL CITATIONS AVAILABLE  
IN THE RE FORMAT

L12 ANSWER 27 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:818975 HCAPLUS

DOCUMENT NUMBER: 134:115941

TITLE: Higher adducts of C<sub>60</sub> by tether-directed remote  
functionalization: X-ray crystal structure and  
reactivity of achiral hexakis-cyclopropanated  
fullerene with all addends located along an  
equatorial belt

AUTHOR(S): Woods, Craig R.; Bourgeois, Jean-Pascal; Seiler,  
Paul; Diederich, Francois

CORPORATE SOURCE: Lab. Organische Chemie, ETH-Zentrum, Zurich,  
8092, Switz.

SOURCE: Angewandte Chemie, International Edition (2000),  
39(21), 3813-3816

CODEN: ACIEF5; ISSN: 1433-7851

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:115941

AB Preparation, crystal structure, and reactivity of a D<sub>2</sub>-sym. hexakis  
adduct are given.

IT 321402-57-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

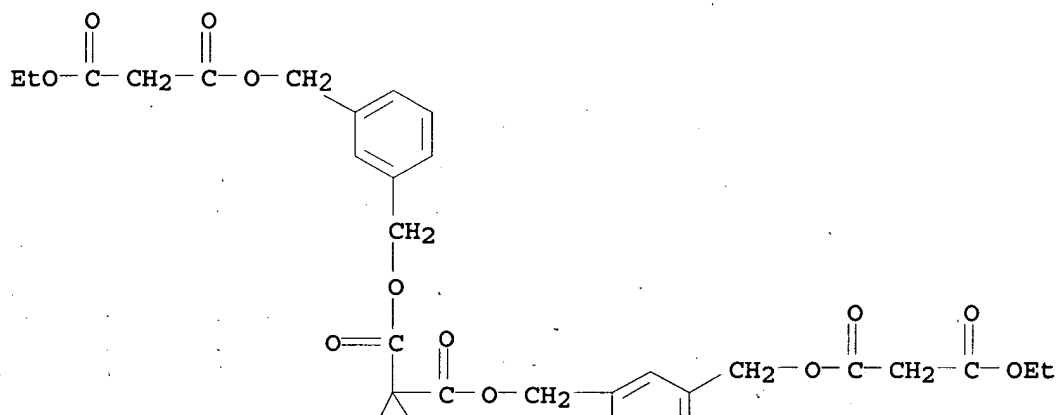
RACT (Reactant or reagent)

(preparation, X-ray crystal structure, and reactivity of achiral hexakis-cyclopropanated fullerene with all addends located along an equatorial belt)

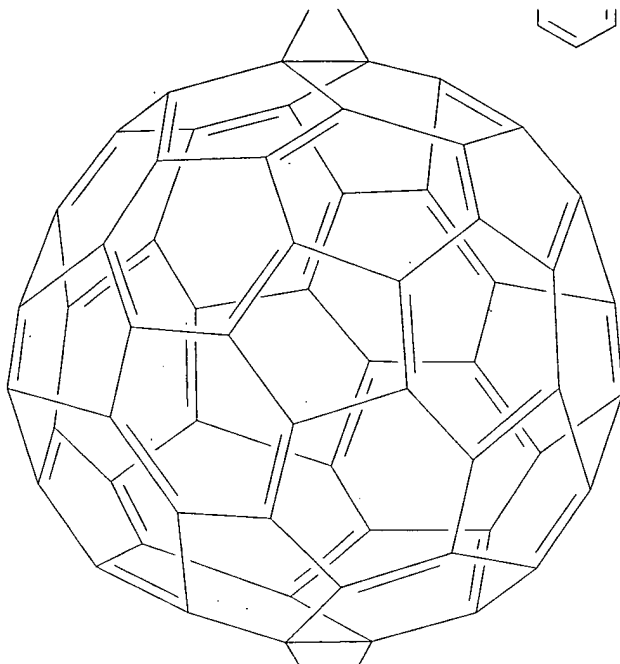
RN 321402-57-7 HCAPLUS

CN 3'H,3''H-Dicyclopropa[1,9:52,60][5,6]fullerene-C60-Ih-3',3',3'',3''-tetracarboxylic acid, tetrakis[3-[(3-ethoxy-1,3-dioxopropoxy)methyl]phenyl]methyl ester (9CI) (CA INDEX NAME)

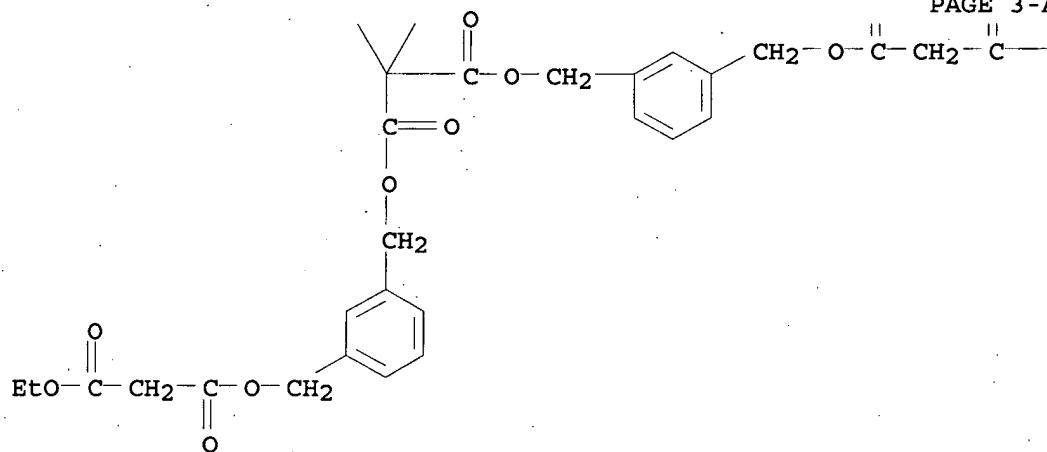
PAGE 1-A



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PAGE 3-B

—OEt

CC 28-23 (Heterocyclic Compounds (More Than One Hetero-Atom))  
 IT 321402-51-1P 321402-53-3P 321402-55-5P 321402-57-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
 RACT (Reactant or reagent)

(preparation, X-ray crystal structure, and reactivity of achiral hexakis-cyclopropanated fullerene with all addends located along an equatorial belt)

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 28 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:481323 HCAPLUS

DOCUMENT NUMBER: 133:237667

TITLE: Selective electrolytic removal of bis(alkoxycarbonyl)methano addends from C60 bis-adducts and electrochemical stability of C70 derivatives

AUTHOR(S): Kessinger, Roland; Fender, Nicolette S.; Echegoyen, Lourdes E.; Thilgen, Carlo; Echegoyen, Luis; Diedrich, Francois

CORPORATE SOURCE: Lab. fur Organische Chemie, ETH-Zentrum, Zurich, 8092, Switz.

SOURCE: Chemistry--A European Journal (2000), 6(12), 2184-2192

CODEN: CEUJED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:237667

AB The novel mixed bis-adducts of C60 with a bis(ethoxycarbonyl)methano addend (Bingel addend) and a second addend ([1,2]benzeno, but[2]eno, methaniminomethano, or diarylmethano) bridging 6,6-closed bonds of the carbon sphere were synthesized in two-step reactions. Each bis-adduct was exhaustively electrolyzed at the potential of the second fullerene-centered reduction step, resulting in the selective removal of the Bingel addend (retro-Bingel reaction) to produce the corresponding mono-adducts, which were isolated in yields of over 60%. These results open up the possibility of using the Bingel addend as a temporary protecting and directing group in the construction of multiple adducts of C60 with unusual addition patterns. The Bingel-type mono-adduct of C70 and constitutionally isomeric bis-adducts were also included in this investigation. A large difference in the electrochem. behavior between C70 bis-adducts and the corresponding C60 derivs. was observed. Thus, the intramol. "walk-on-the-sphere" isomerization which occurs readily with Bingel-type bis-adducts of C60 under the conditions of two-electron controlled potential electrolysis (CPE) is only a minor reaction pathway in the series of C70 derivs. The later preferentially undergo retro-Bingel reaction.

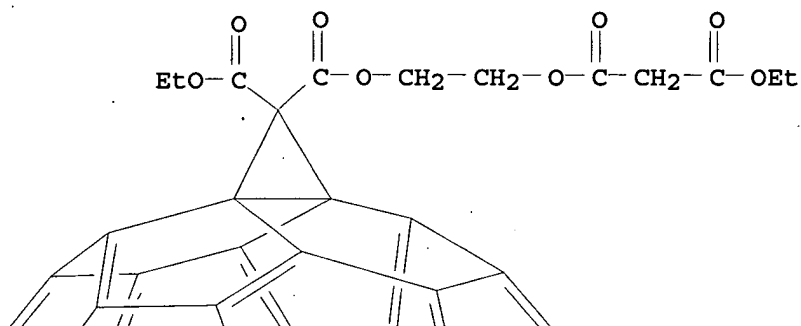
IT 293768-14-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(electrochem. retro-Bingel reaction of fullerene adducts)

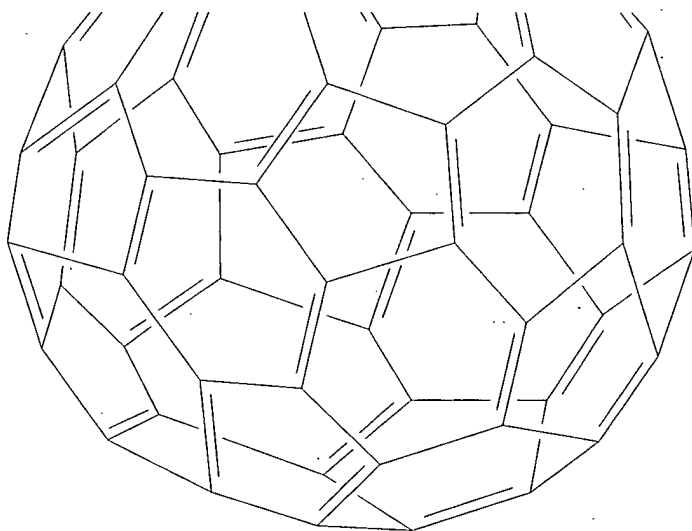
RN 293768-14-6 HCAPLUS

CN 3'H-Cyclopropa[1,9][5,6]fullerene-C60-1h-3',3'-dicarboxylic acid, 2-(3-ethoxy-1,3-dioxopropoxy)ethyl ethyl ester (9CI) (CA INDEX NAME)

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CC 25-29 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT 115383-22-7P, C70 Fullerene 154133-70-7P 293768-14-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(electrochem. retro-Bingel reaction of fullerene adducts)

REFERENCE COUNT: 75 THERE ARE 75 CITED REFERENCES AVAILABLE  
FOR THIS RECORD. ALL CITATIONS AVAILABLE  
IN THE RE FORMAT

L12 ANSWER 29 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:727152 HCAPLUS

DOCUMENT NUMBER: 128:75385

TITLE: Macrocyclization on the fullerene core. Direct regio- and diastereoselective multi-functionalization of [60]fullerene, and synthesis of fullerene-dendrimer derivatives

AUTHOR(S): Nierengarten, Jean Francois; Habicher, Tilo; Kessinger, Roland; Cardullo, Francesca; Diederich, Francois; Gramlich, Volker; Gisselbrecht, Jean Paul; Boudon, Corinne; Gross, Maurice

CORPORATE SOURCE: Lab. Organische Chem., ETH-Zentrum, Zurich, CH-8092, Switz.

SOURCE: Helvetica Chimica Acta (1997), 80(7), 2238-2276  
CODEN: HCACAV; ISSN: 0018-019X

PUBLISHER: Verlag Helvetica Chimica Acta

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 128:75385

AB The macrocyclization between buckminsterfullerene, C<sub>60</sub>, and bis-malonate derivs. in a double Bingel reaction provides a versatile and simple method for the preparation of covalent bis-adducts of C<sub>60</sub> with high regio- and diastereoselectivity. A combination of spectral anal., stereochem. considerations, and x-ray crystallog. revealed that out of the possible in-in, in-out, and out-out stereoisomers, the reaction of bis-malonates linked by 1,2-, 1,3-, or 1,4-xylylene tethers afforded only the out-out ones. In contrast, the use of larger tethers derived from 1,10-phenanthroline also provided a first example of an in-out product. Starting from optically pure bis-malonate derivs., the new bis-functionalization method permitted the diastereoselective preparation of optically active fullerene derivs. and, ultimately, the enantioselective preparation (>97% ee) of optically active cis-3 bis-adducts whose chirality results exclusively from the addition pattern. The macrocyclic fixation of a bis-malonate with an optically active, 9,9'-spirobi[9H-fluorene]-derived tether to C<sub>60</sub> under generation of a bis-adduct with an achiral addition pattern induces dramatic changes in the chiroptical properties of the tether chromophore such as strong enhancement and reversal of sign of the Cotton effects in the CD spectra. By the same method, functionalized bis-adducts were prepared as initiator cores for the synthesis of fullerene dendrimers by convergent growth. Finally, the new methodol. was extended to the regio- and diastereoselective construction of higher cyclopropanated adducts. Electrochem. investigations by steady-state voltammetry in CH<sub>2</sub>Cl<sub>2</sub> showed that all macrocyclic bis(methano)fullerenes underwent multiple reduction steps, and that regioisomerism was not much influencing the redox potentials. All cis-2 bis-adducts gave an instable dianion which decomposed during the electrochem. reduction. In CH<sub>2</sub>Cl<sub>2</sub>, the redox potential of the fullerene core in the dendrimers is not affected by differences in size and d. of the surrounding poly(ether-amide) dendrons. All-cis-2 tris- and tetrakis(methano)fullerenes are reduced at more neg. potential than previously reported all-e tris- and tetrakis-adducts with methano bridges that are also located along an equatorial belt. This indicates a larger perturbation of the original fullerene  $\pi$ -chromophore and a larger raise in LUMO energy in the former derivs.

IT 200353-32-8P



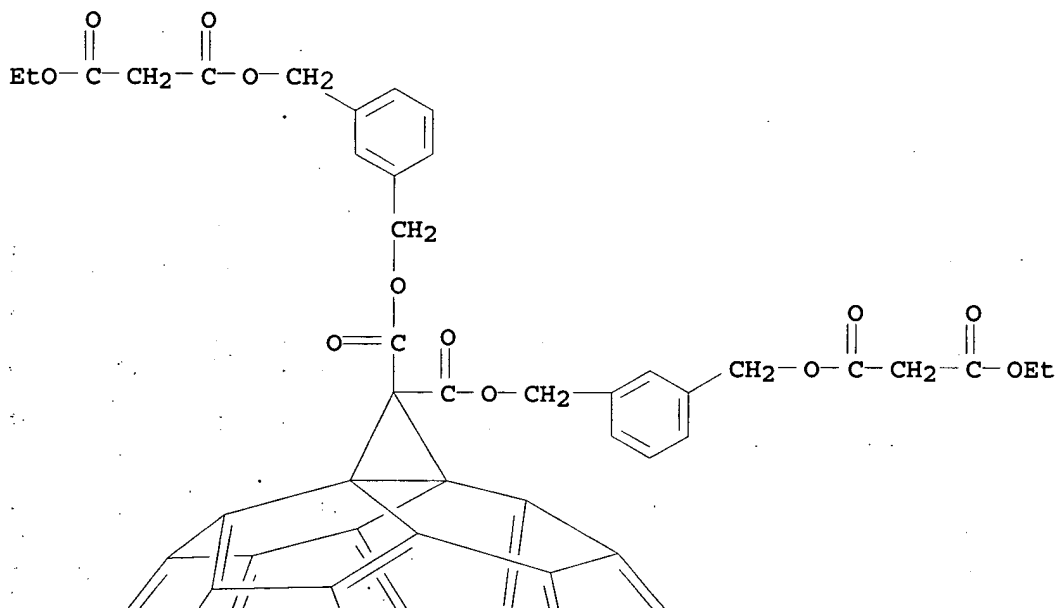
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
RACT (Reactant or reagent)

(preparation of fullerene dendrimers and multifunctionalized  
fullerenes by macrocyclization on fullerene core and redox  
properties thereof)

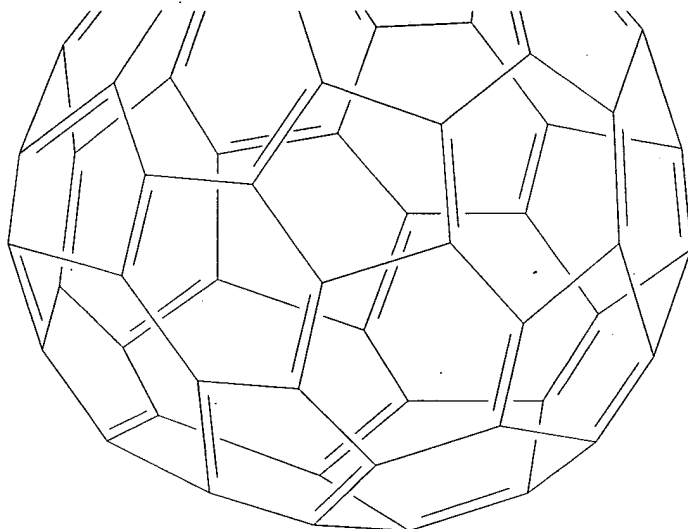
RN 200353-32-8 HCAPLUS

CN 3'H-Cyclopropa[1,9][5,6]fullerene-C60-1h-3',3'-dicarboxylic acid,  
bis[[3-[(3-ethoxy-1,3-dioxopropoxy)methyl]phenyl]methyl] ester (9CI)  
(CA INDEX NAME)

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CC 28-23 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 22

IT 56-40-6DP, Glycine, dendrimer-bound, preparation 1138-80-3DP,  
dendrimer-bound 175724-30-8P 184414-50-4P 184414-52-6P

184414-54-8P 200133-12-6P 200133-13-7P 200133-14-8P

200133-15-9P 200133-16-0P 200133-17-1P 200133-18-2P

200133-19-3P 200133-20-6P 200133-21-7P 200133-23-9P

200133-24-0P 200133-25-1P 200133-26-2P 200133-27-3P

200133-28-4P 200133-29-5P 200133-30-8P 200133-31-9P

200133-32-0P 200352-99-4P 200353-10-2P 200353-14-6P

200353-15-7P 200353-17-9P 200353-20-4P 200353-30-6P

200353-32-8P 200353-34-0P 200353-36-2P 200353-37-3P

200353-39-5P 200353-40-8P 200443-74-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
RACT (Reactant or reagent)(preparation of fullerene dendrimers and multifunctionalized  
fullerenes by macrocyclization on fullerene core and redox  
properties thereof)

L12 ANSWER 30 OF 30 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:204019 HCAPLUS

DOCUMENT NUMBER: 126:186117

TITLE: Fullerene derivatives, process for their  
regioselective preparation, and their use in  
electrooptical components.

INVENTOR(S): Bingel, Carsten

PATENT ASSIGNEE(S): Hoechst A.-G., Germany

SOURCE: Ger. Offen., 13 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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DE 19526173 A1 19970130 DE 1995-19526173

199507  
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WO 9703975 A1 19970206 WO 1996-EP2960

199607  
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W: CA, JP, US

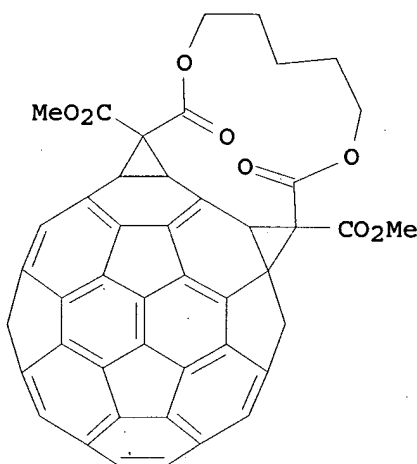
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,  
PT, SE

PRIORITY APPLN. INFO.:

DE 1995-19526173 A

199507  
18OTHER SOURCE(S):  
GI

CASREACT 126:186117; MARPAT 126:186117



, II

AB Bridged, bis-cyclopropanated fullerenes of formula  
 $E1C(:Full)E2XE3C(:Full)E4$  [I; (:Full) = cyclopropa fusion to C<sub>24</sub>-220  
 fullerene; E<sub>1</sub>, E<sub>4</sub> = H, COR, CO<sub>2</sub>H and derivs., SO<sub>2</sub>R, NO<sub>2</sub>, etc.; E<sub>2</sub>,  
 E<sub>3</sub> = COO, CONR, CO, P(O)(OR)O, SO<sub>2</sub>; X = variety of bridging groups]  
 are claimed, and are useful in the preparation of electrooptical  
 components (no data). I are prepared in a simple one-pot reaction  
 with a high degree of regioselectivity. For instance, C<sub>60</sub> in PhMe  
 reacted with the bis(malonate) MeO<sub>2</sub>CCH<sub>2</sub>CO<sub>2</sub>XO<sub>2</sub>CCH<sub>2</sub>CO<sub>2</sub>Me [X = (CH<sub>2</sub>)<sub>5</sub>]  
 upon treatment with I<sub>2</sub> and then DBU, giving 35% of the cis-2  
 regioisomer II. Similar reactions of C<sub>60</sub> with other bis(malonates)  
 [X = CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>-p, (CH<sub>2</sub>)<sub>n</sub> (n = 2, 3, 4, 6, 7, 8)] each gave 1-3  
 regioisomers of I in 7-60% combined yields.

IT 187663-37-2P 187663-39-4P

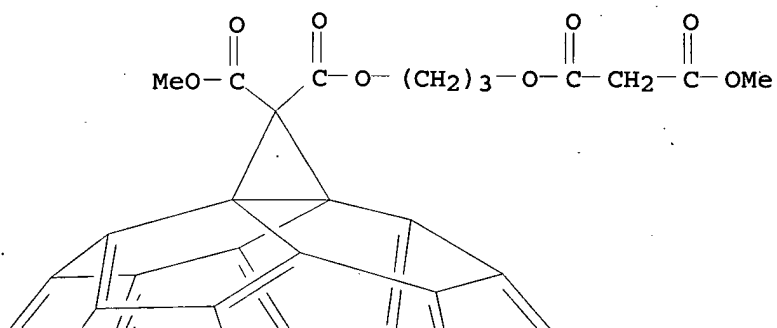
RL: BYP (Byproduct); PREP (Preparation)

(byproduct; preparation of bridged fullerene derivs. by regioselective  
 biscyclopropanation of C<sub>60</sub> with bis(malonates))

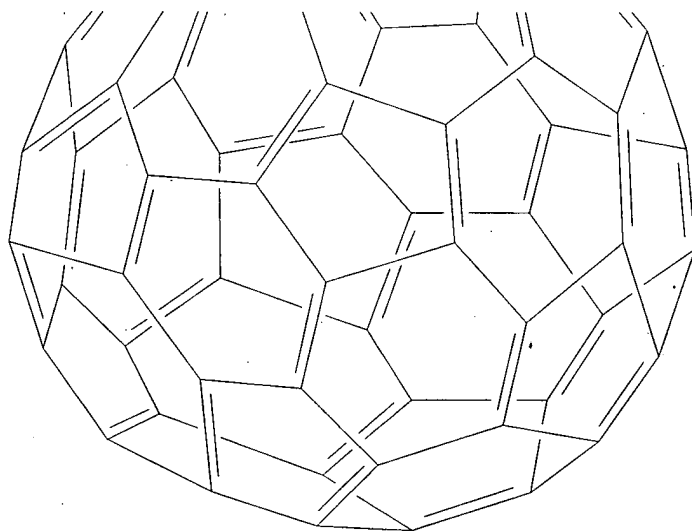
RN 187663-37-2 HCAPLUS

CN 3'H-Cyclopropa[1,9][5,6]fullerene-C<sub>60</sub>-1h-3',3'-dicarboxylic acid,  
 3-(3-methoxy-1,3-dioxopropoxy)propyl methyl ester (9CI) (CA INDEX  
 NAME)

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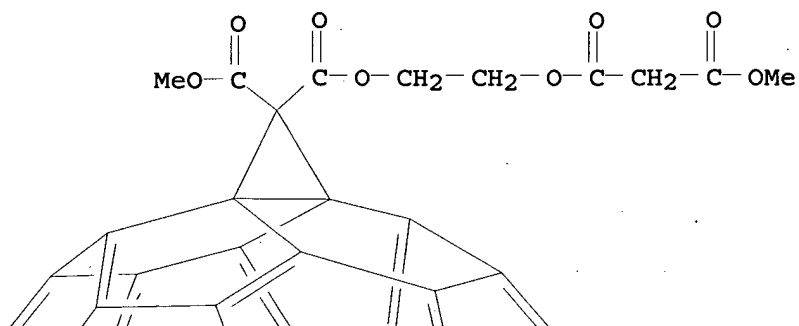


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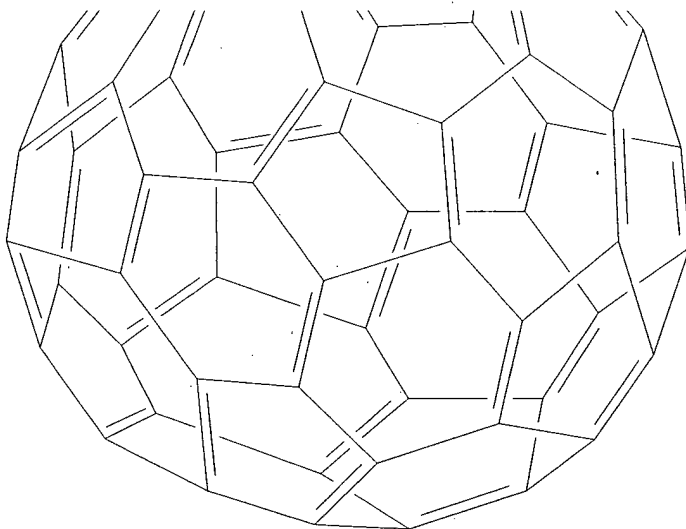


RN 187663-39-4 HCAPLUS  
 CN 3'H-Cyclopropa[1,9][5,6]fullerene-C60-Ih-3',3'-dicarboxylic acid,  
 2-(3-methoxy-1,3-dioxopropoxy)ethyl methyl ester (9CI) (CA INDEX  
 NAME)

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IC ICM C07D321-10  
ICS C07D245-04; C07F009-40; C07F009-6574; C07F007-08; C07B053-00;  
C01B031-00  
ICA C07C069-38  
ICI C07M009-00  
CC 28-23 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 73, 76

IT 187663-37-2P 187663-39-4P

RL: BYP (Byproduct); PREP (Preparation)

(byproduct; preparation of bridged fullerene derivs. by regioselective  
• biscyclopropanation of C60 with bis(malonates))

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